



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:46 pm GMT

PDB ID : 5MMM
EMDB ID : EMD-3533
Title : Structure of the 70S chloroplast ribosome
Authors : Bieri, P.; Leibundgut, M.; Saurer, M.; Boehringer, D.; Ban, N.
Deposited on : 2016-12-11
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

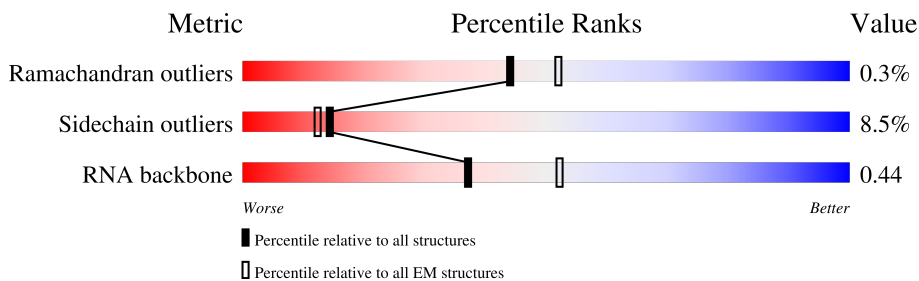
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















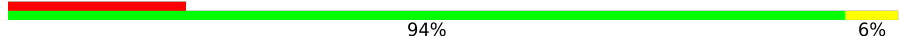










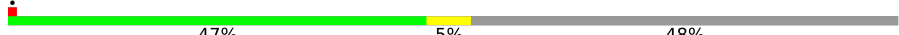
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	130	
2	1	57	
3	2	66	
4	3	152	
5	4	159	
6	5	37	
7	6	142	
8	7	116	


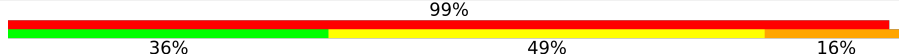
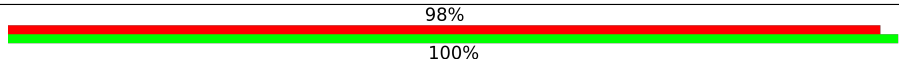
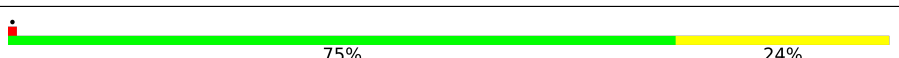
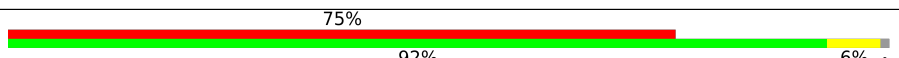
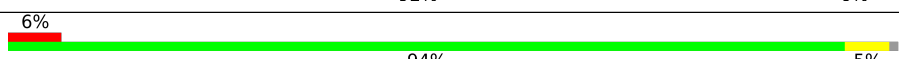
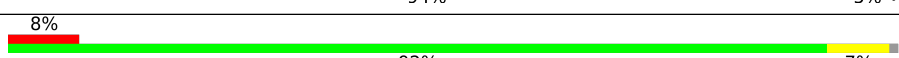
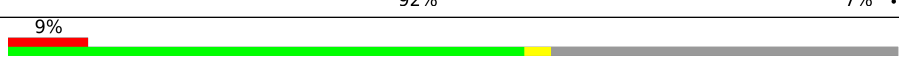

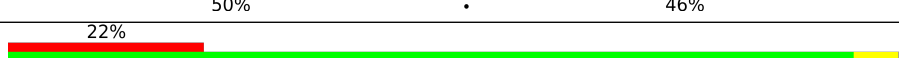
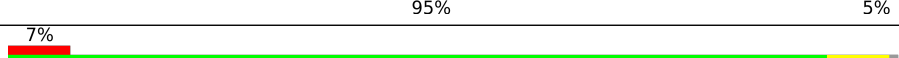
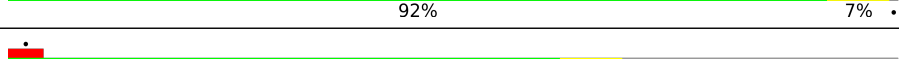
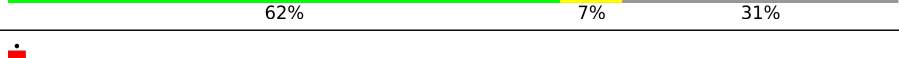


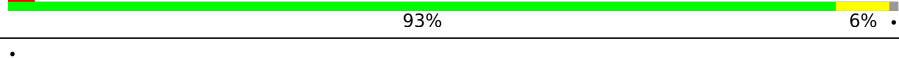

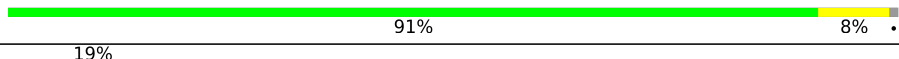
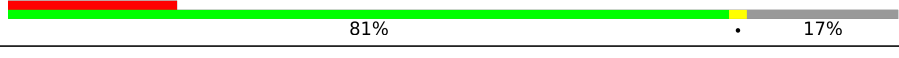

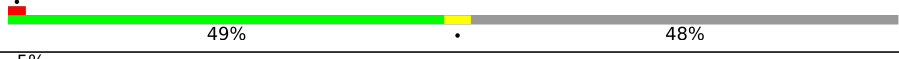




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Mol	Chain	Length	Quality of chain
9	A	2810	
10	B	121	
11	C	272	
12	D	305	
13	E	293	
14	F	258	
15	G	220	
16	H	196	
17	I	232	
18	J	224	
19	K	250	
20	L	121	
21	M	271	
22	N	135	
23	O	126	
24	P	166	
25	Q	233	
26	R	128	
27	S	256	
28	T	199	
29	U	198	
30	V	192	
31	W	106	
32	X	194	
33	Y	148	

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Mol	Chain	Length	Quality of chain
34	Z	168	
35	z	76	
36	8	174	
37	a	1491	
38	b	236	
39	c	218	
40	d	201	
41	e	308	
42	f	211	
43	g	155	
44	h	134	
45	i	208	
46	j	195	
47	k	138	
48	l	123	
49	m	172	
50	n	100	
51	o	90	
52	p	88	
53	q	165	
54	r	101	
55	s	92	
56	t	183	
57	u	180	
58	v	260	

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Mol	Chain	Length	Quality of chain
59	w	179	37% 46% 54%
60	x	101	40% 60%
61	y	302	37% 62%

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 152465 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	66	536	338	94	102	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	48	396	261	75	60	0	0

- Molecule 3 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	60	489	304	98	83	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	60	467	282	107	75	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	72	588	370	124	93	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	37	305	186	70	45	4	0	0

- Molecule 7 is a protein called plastid ribosomal protein cL37, PSRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	49	422	268	92	57	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	46	368	237	71	59	1	0	0

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A	2798	60083	26804	11116	19365	2798	0	0

- Molecule 10 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B	121	2584	1154	466	843	121	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	253	1952	1209	401	336	6	0	0

- Molecule 12 is a protein called plastid ribosomal protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	221	1686	1066	308	301	11	0	0

- Molecule 13 is a protein called plastid ribosomal protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	212	1676	1061	312	300	3	0	0

- Molecule 14 is a protein called plastid ribosomal protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	193	1454	923	255	268	8	0	0

- Molecule 15 is a protein called plastid ribosomal protein uL6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	178	1391	878	256	253	4	0	0

- Molecule 16 is a protein called plastid ribosomal protein bL9c.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	H	48	382	251	69	62	0	0

- Molecule 17 is a protein called plastid ribosomal protein uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	137	1106	711	186	203	6	0	0

- Molecule 18 is a protein called 50S ribosomal protein L11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	133	977	624	161	186	6	0	0

- Molecule 19 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	203	1648	1047	307	289	5	0	0

- Molecule 20 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	121	942	588	179	170	5	0	0

- Molecule 21 is a protein called plastid ribosomal protein uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	185	Total	C	N	O	S	0	0
			1410	879	280	245	6		

- Molecule 22 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	135	Total	C	N	O	S	0	0
			1075	677	218	174	6		

- Molecule 23 is a protein called plastid ribosomal protein uL14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 24 is a protein called plastid ribosomal protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	122	Total	C	N	O	S	0	0
			962	598	186	173	5		

- Molecule 25 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	118	Total	C	N	O	S	0	0
			953	611	186	155	1		

- Molecule 26 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	119	Total	C	N	O	S	0	0
			1029	652	213	162	2		

- Molecule 27 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	S	170	Total	C	N	O	0	0
			1310	844	227	239		

- Molecule 28 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	172	Total	C	N	O	S	0	0
			1395	892	257	237	9		

- Molecule 29 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	96	Total	C	N	O	S	0	0
			776	503	135	136	2		

- Molecule 30 is a protein called plastid ribosomal protein uL24c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	134	Total	C	N	O	S	0	0
			1078	677	203	195	3		

- Molecule 31 is a RNA chain called 4.5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	106	Total	C	N	O	P	0	0
			2277	1017	423	731	106		

- Molecule 32 is a protein called plastid ribosomal protein bL27c.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	109	Total	C	N	O	0	0
			888	560	175	153		

- Molecule 33 is a protein called plastid ribosomal protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	77	Total	C	N	O	S	0	0
			634	402	128	103	1		

- Molecule 34 is a protein called plastid ribosomal protein uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	101	Total	C	N	O	S	0	0
			846	529	167	147	3		

- Molecule 35 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	z	76	1623	723	290	534	76	0	0

- Molecule 36 is a protein called plastid ribosomal protein bS1c.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	8	174	870	522	174	174	0	0

- Molecule 37 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	a	1484	31868	14208	5881	10295	1484	0	0

- Molecule 38 is a protein called 30S ribosomal protein S2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	b	233	1844	1163	339	329	13	0	0

- Molecule 39 is a protein called 30S ribosomal protein S3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	c	216	1736	1108	313	309	6	0	0

- Molecule 40 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	d	199	1633	1032	319	278	4	0	0

- Molecule 41 is a protein called 30S ribosomal protein S5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	e	187	1331	826	259	240	6	0	0

- Molecule 42 is a protein called plastid ribosomal protein bS6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	f	113	911	583	152	172	4	0	0

- Molecule 43 is a protein called 30S ribosomal protein S7, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	g	154	1210	753	244	210	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	h	133	1079	679	210	185	5	0	0

- Molecule 45 is a protein called plastid ribosomal protein uS9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	i	144	1119	712	211	195	1	0	0

- Molecule 46 is a protein called plastid ribosomal protein uS10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	j	99	805	517	144	139	5	0	0

- Molecule 47 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	k	117	882	546	181	150	5	0	0

- Molecule 48 is a protein called 30S ribosomal protein S12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	l	122	959	599	197	161	2	0	0

- Molecule 49 is a protein called plastid ribosomal protein uS13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	m	110	Total	C	N	O	S	0	0
			904	556	182	161	5		

- Molecule 50 is a protein called 30S ribosomal protein S14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	n	99	Total	C	N	O	S	0	0
			820	507	174	136	3		

- Molecule 51 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	o	75	Total	C	N	O	S	0	0
			635	404	123	107	1		

- Molecule 52 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	p	80	Total	C	N	O	S	0	0
			664	425	123	114	2		

- Molecule 53 is a protein called plastid ribosomal protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	q	86	Total	C	N	O	S	0	0
			693	434	136	119	4		

- Molecule 54 is a protein called 30S ribosomal protein S18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	r	60	Total	C	N	O	S	0	0
			490	308	96	85	1		

- Molecule 55 is a protein called 30S ribosomal protein S19 alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	s	78	Total	C	N	O	S	0	0
			631	406	119	104	2		

- Molecule 56 is a protein called plastid ribosomal protein bS20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	t	107	Total	C	N	O	S	0	0
			853	528	173	151	1		

- Molecule 57 is a protein called plastid ribosomal protein bS21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	u	65	Total	C	N	O	S	0	0
			568	339	127	100	2		

- Molecule 58 is a protein called 30S ribosomal protein 2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	v	80	Total	C	N	O	0	0
			613	388	104	121		

- Molecule 59 is a protein called 30S ribosomal protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	w	82	Total	C	N	O	S	0	0
			686	454	113	116	3		

- Molecule 60 is a protein called 30S ribosomal protein S31, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	x	40	Total	C	N	O	0	0
			309	192	69	48		

- Molecule 61 is a protein called Ribosome-binding factor PSRP1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	y	116	Total	C	N	O	S	0	0
			919	567	181	169	2		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	2	1	Total	Zn	0
			1	1	
62	5	1	Total	Zn	0
			1	1	

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
63	4	1	Total Mg 1 1	0
63	6	1	Total Mg 1 1	0
63	7	1	Total Mg 1 1	0
63	A	511	Total Mg 511 511	0
63	B	15	Total Mg 15 15	0
63	C	1	Total Mg 1 1	0
63	D	1	Total Mg 1 1	0
63	E	1	Total Mg 1 1	0
63	F	1	Total Mg 1 1	0
63	H	1	Total Mg 1 1	0
63	M	2	Total Mg 2 2	0
63	P	1	Total Mg 1 1	0
63	R	1	Total Mg 1 1	0
63	S	1	Total Mg 1 1	0
63	T	1	Total Mg 1 1	0
63	U	1	Total Mg 1 1	0
63	V	1	Total Mg 1 1	0
63	W	14	Total Mg 14 14	0
63	a	219	Total Mg 219 219	0
63	k	1	Total Mg 1 1	0
63	l	1	Total Mg 1 1	0
63	n	1	Total Mg 1 1	0

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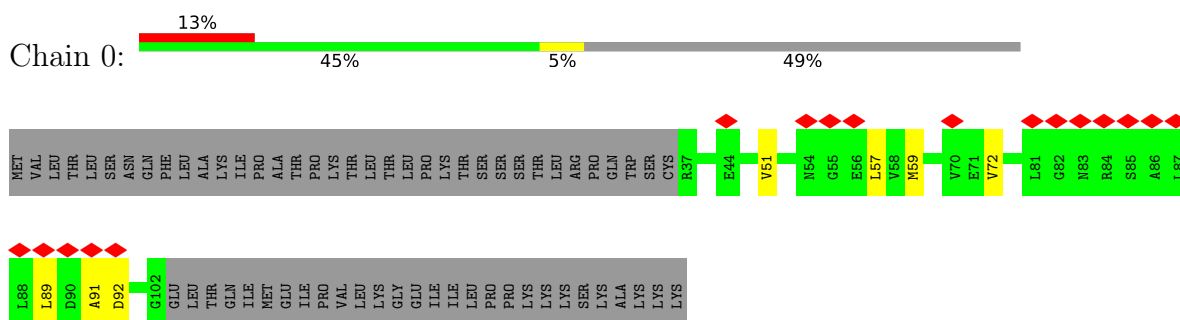
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
63	x	1	1	1	0

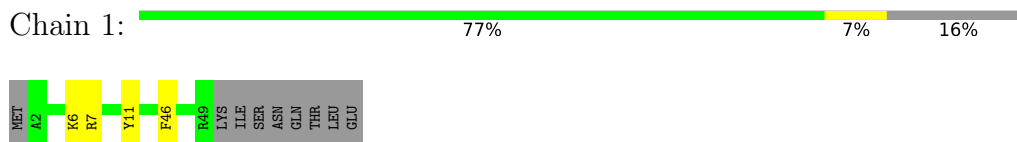
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

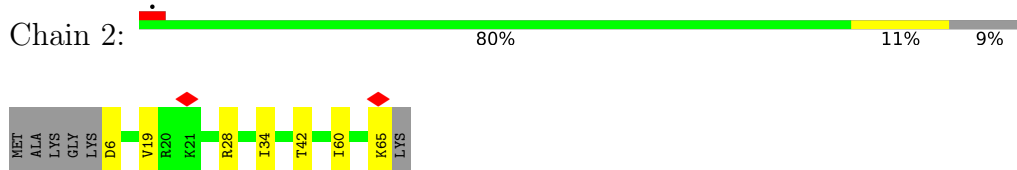
- Molecule 1: 50S ribosomal protein L31



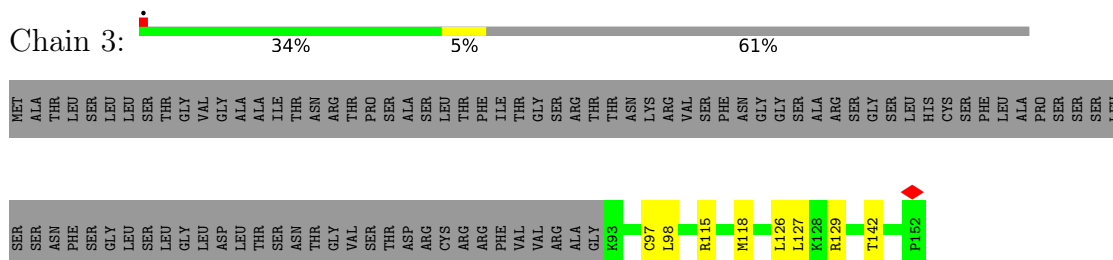
- Molecule 2: 50S ribosomal protein L32, chloroplastic



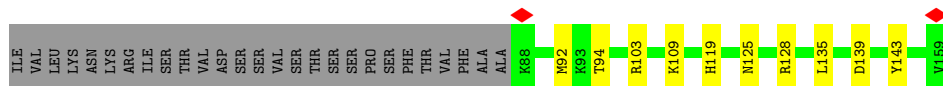
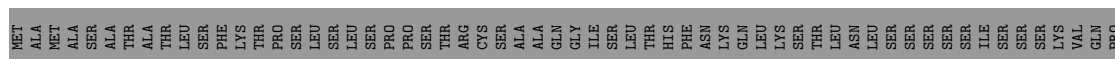
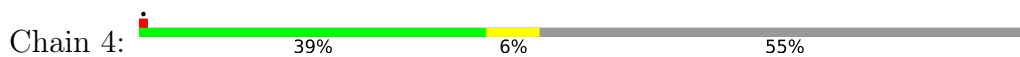
- Molecule 3: 50S ribosomal protein L33, chloroplastic



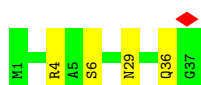
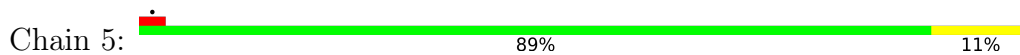
- Molecule 4: 50S ribosomal protein L34, chloroplastic



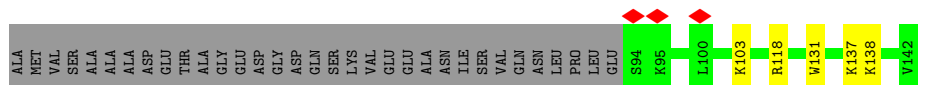
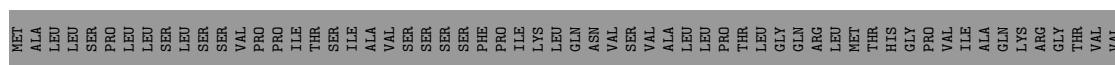
- Molecule 5: 50S ribosomal protein L35, chloroplastic



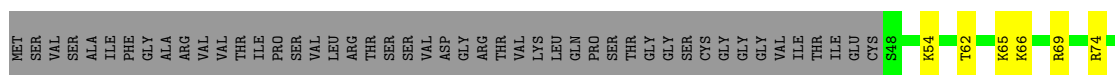
● Molecule 6: 50S ribosomal protein L36, chloroplastic



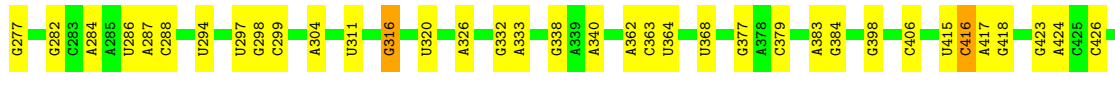
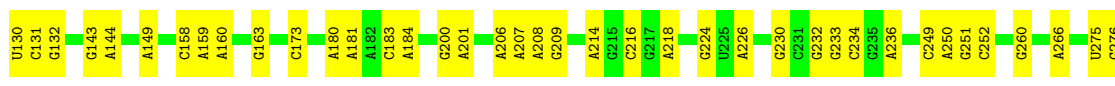
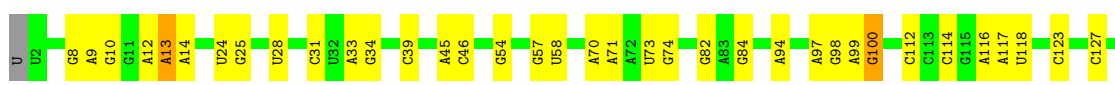
● Molecule 7: plastid ribosomal protein cL37, PSRP5

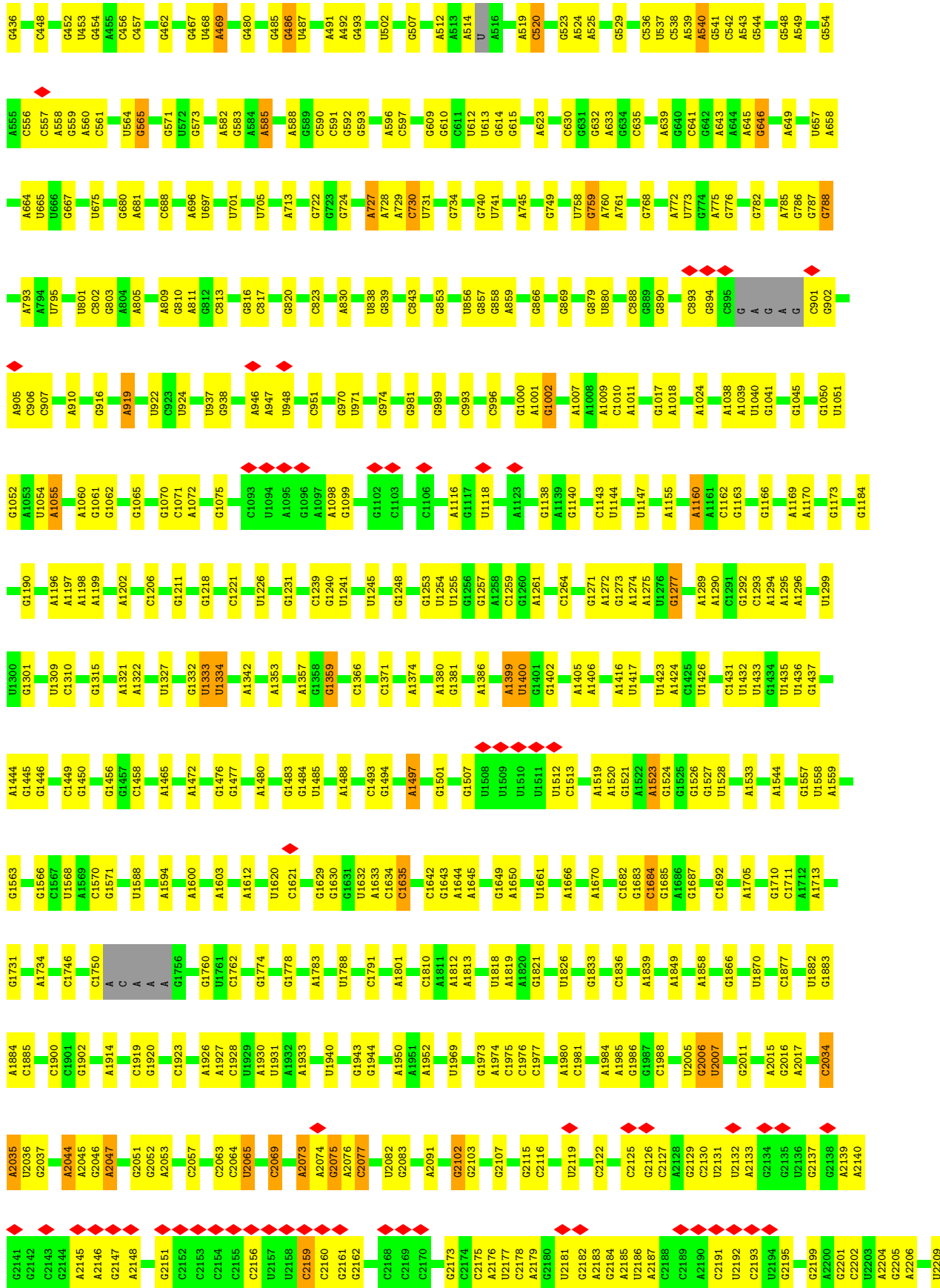


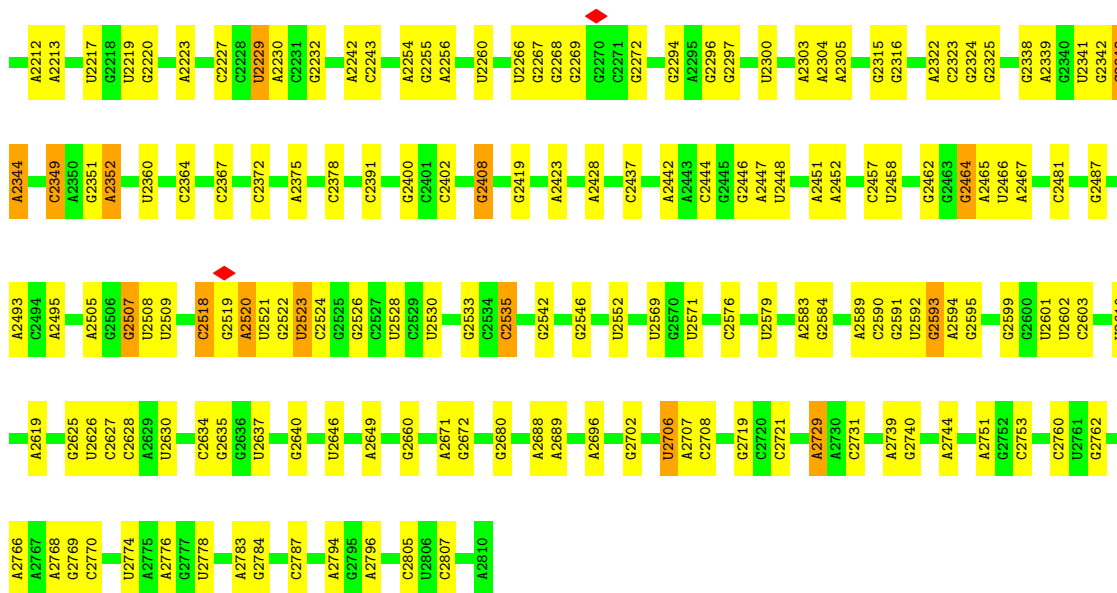
● Molecule 8: 50S ribosomal protein 6, chloroplastic



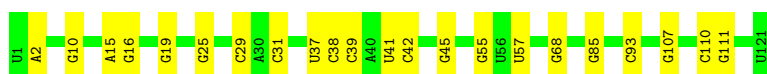
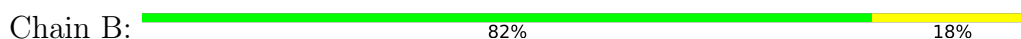
● Molecule 9: 23S ribosomal RNA



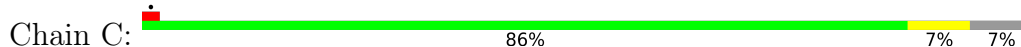




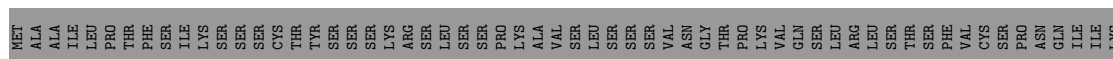
● Molecule 10: 5S ribosomal RNA



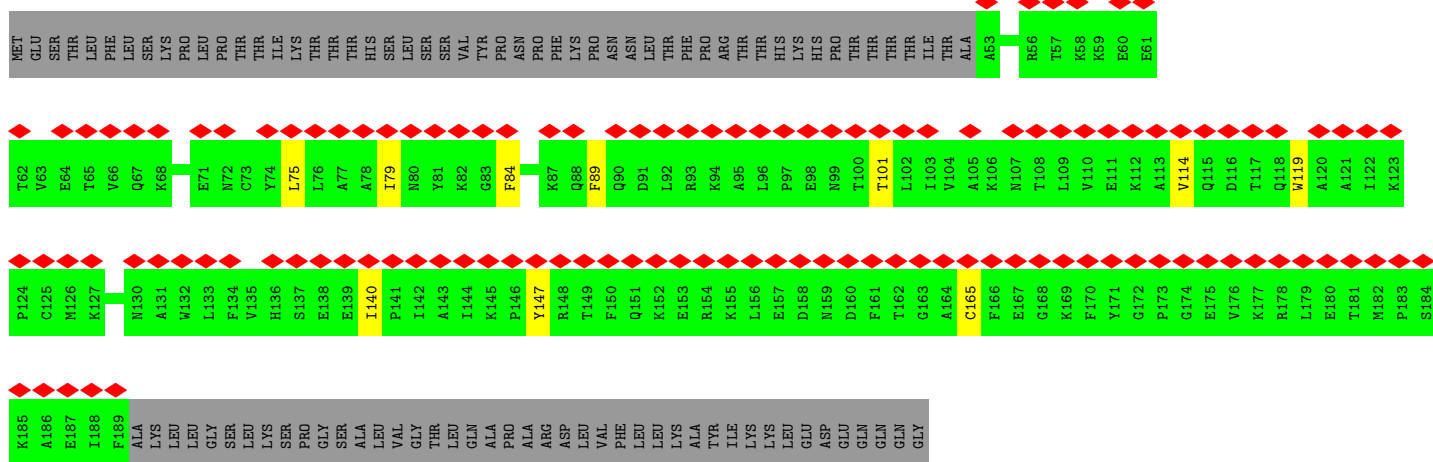
● Molecule 11: 50S ribosomal protein L2, chloroplastic



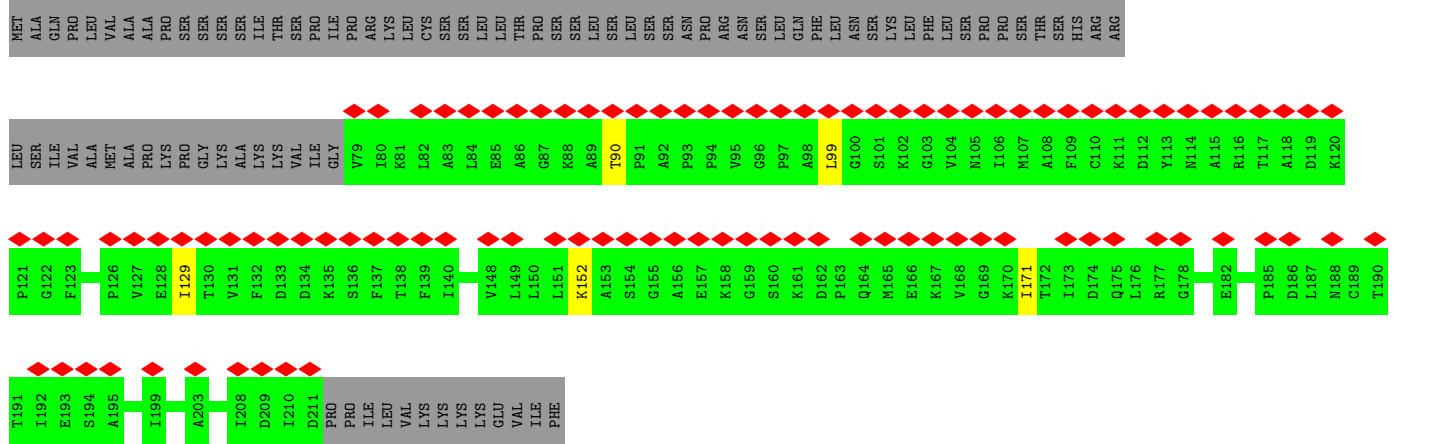
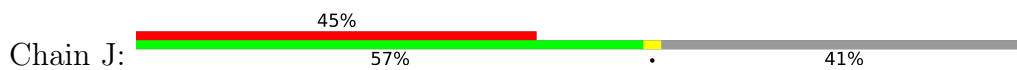
● Molecule 12: plastid ribosomal protein uL3c



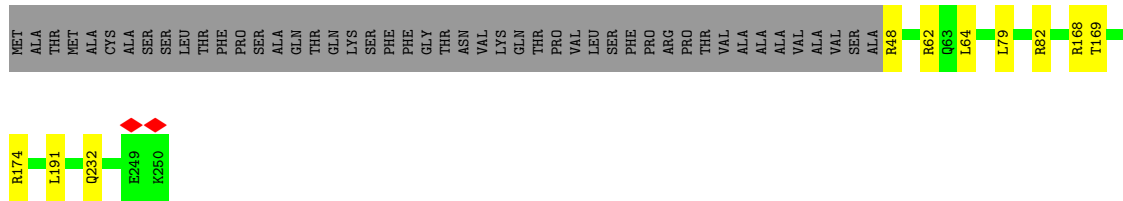
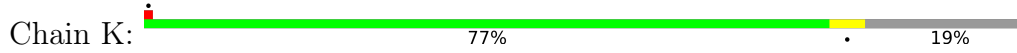
● Molecule 13: plastid ribosomal protein uL4c



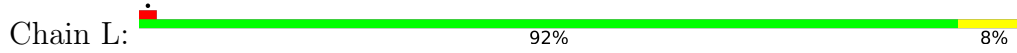
• Molecule 18: 50S ribosomal protein L11, chloroplastic

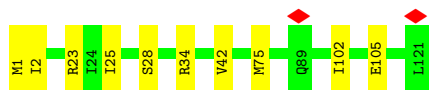


• Molecule 19: 50S ribosomal protein L13, chloroplastic

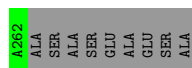


• Molecule 20: 50S ribosomal protein L14, chloroplastic

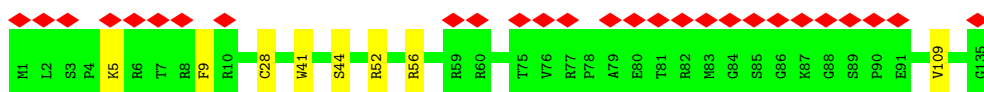




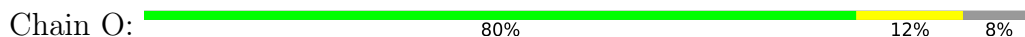
• Molecule 21: plastid ribosomal protein uL15c



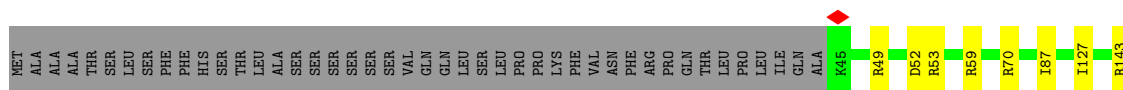
• Molecule 22: 50S ribosomal protein L16, chloroplastic



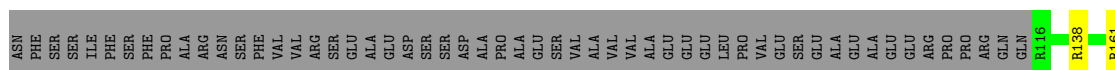
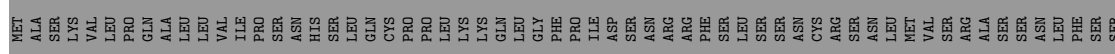
• Molecule 23: plastid ribosomal protein uL14c



• Molecule 24: plastid ribosomal protein uL18c

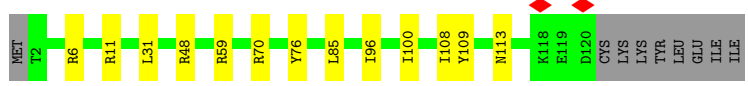
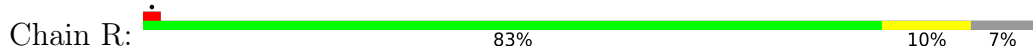


• Molecule 25: 50S ribosomal protein L19, chloroplastic

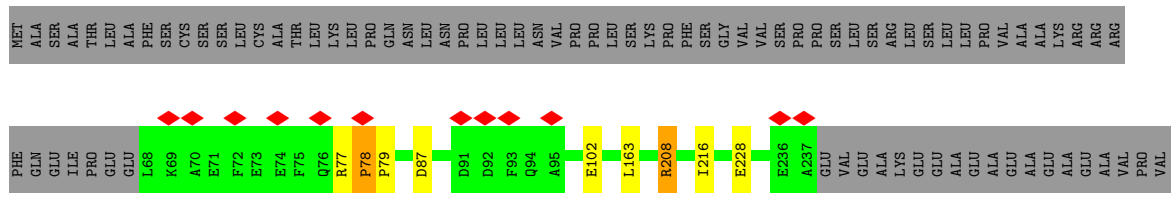




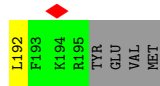
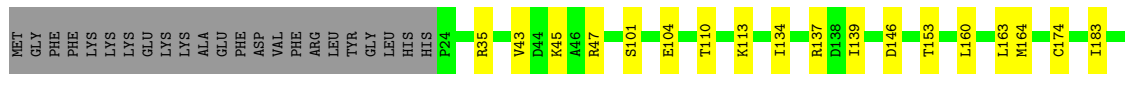
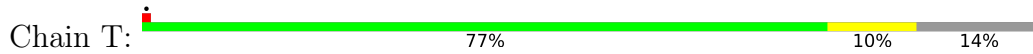
● Molecule 26: 50S ribosomal protein L20, chloroplastic



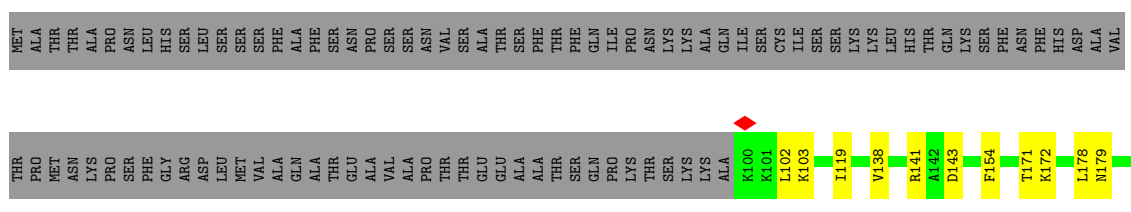
● Molecule 27: 50S ribosomal protein L21, chloroplastic



● Molecule 28: 50S ribosomal protein L22, chloroplastic

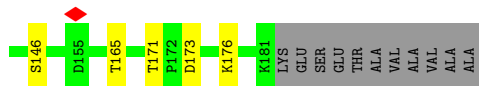
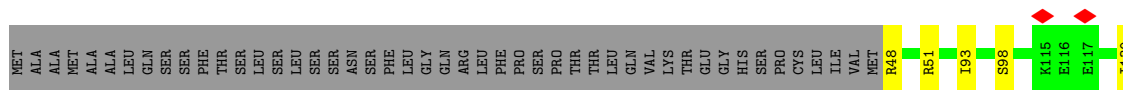


● Molecule 29: 50S ribosomal protein L23, chloroplastic

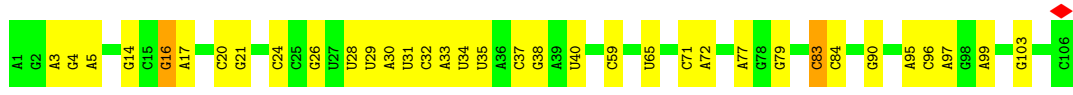


● Molecule 30: plastid ribosomal protein uL24c

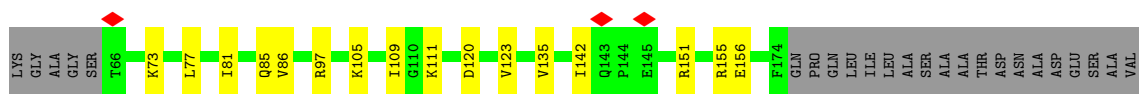
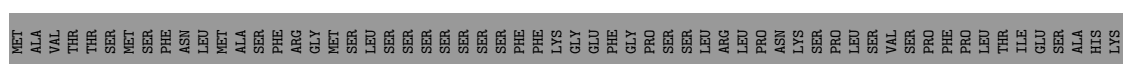




• Molecule 31: 4.5S ribosomal RNA

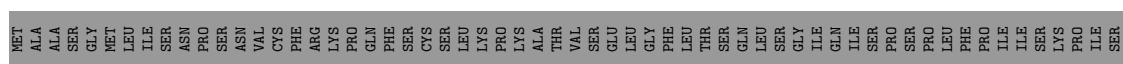


• Molecule 32: plastid ribosomal protein bL27c

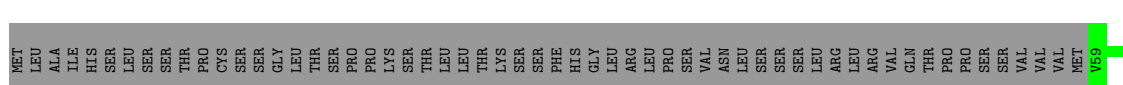


CYS

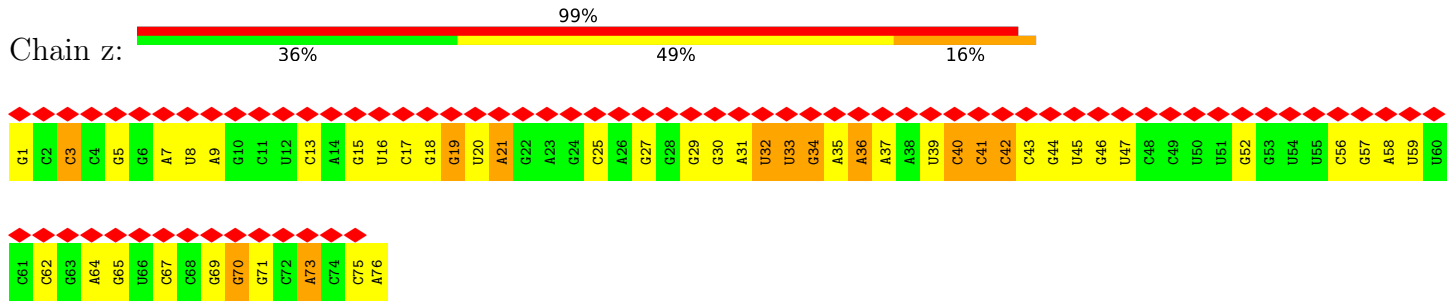
• Molecule 33: plastid ribosomal protein bL28c



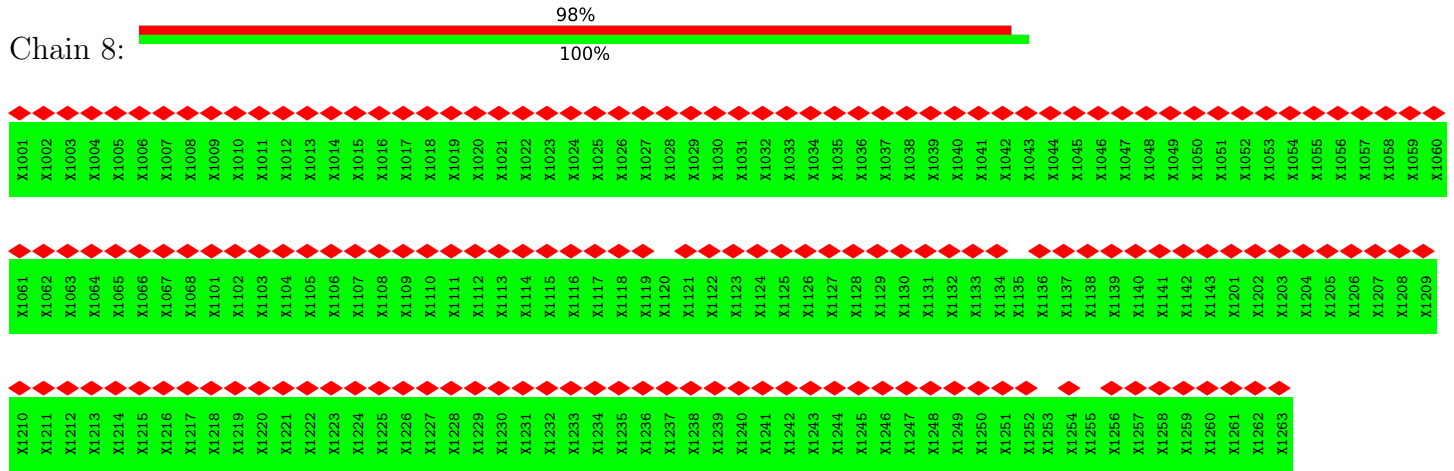
• Molecule 34: plastid ribosomal protein uL29c



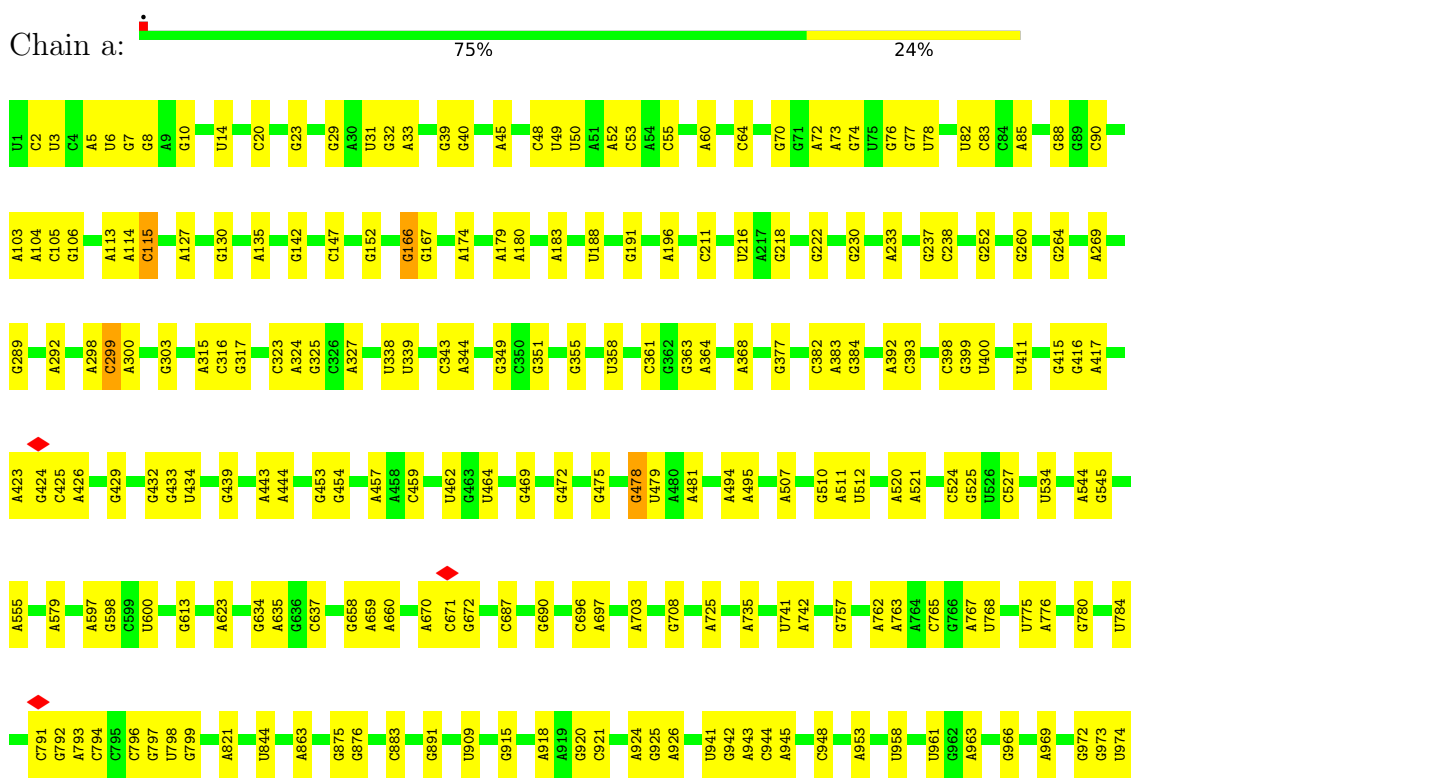
• Molecule 35: tRNA-Phe

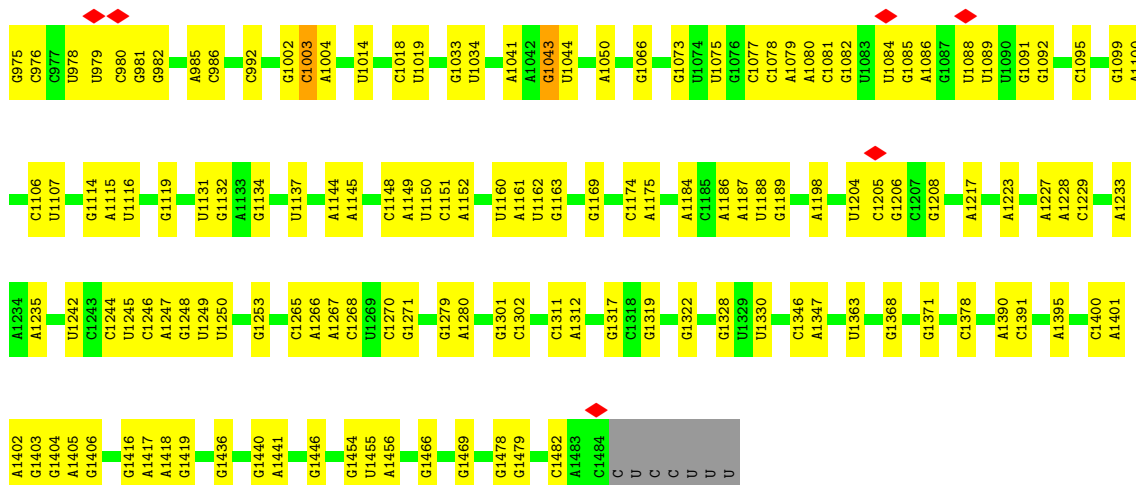


• Molecule 36: plastid ribosomal protein bS1c

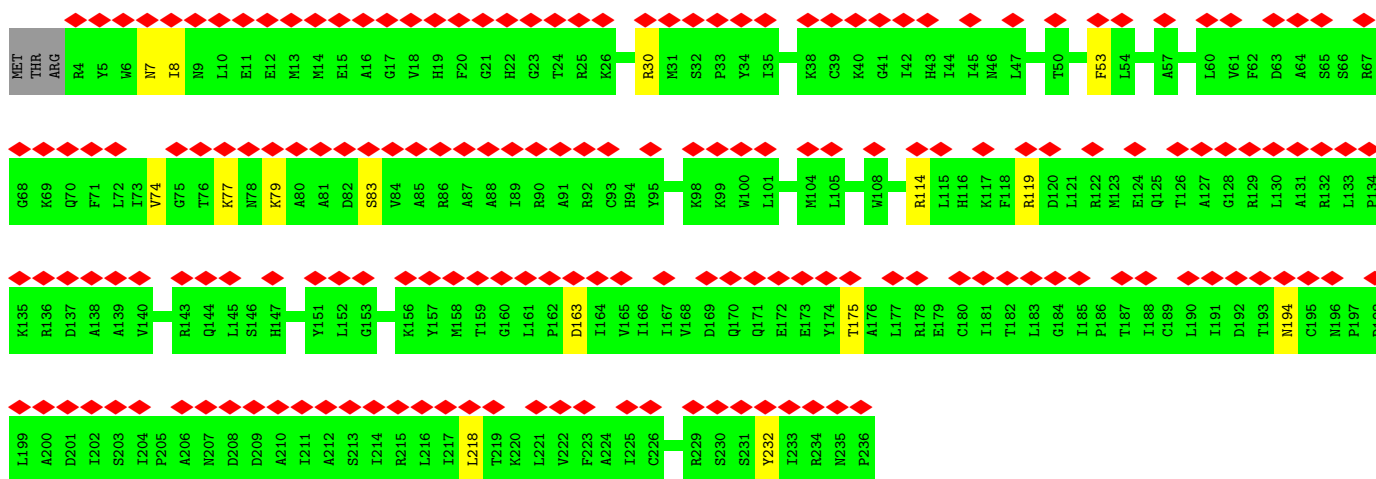
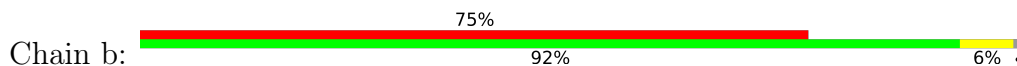


• Molecule 37: 16S ribosomal RNA

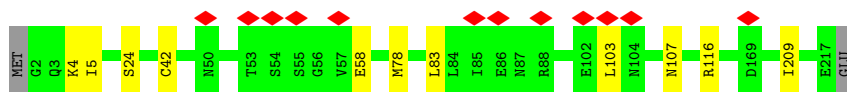
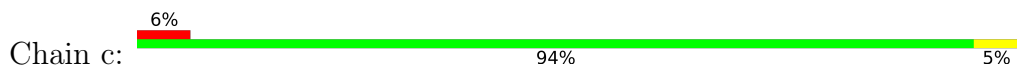




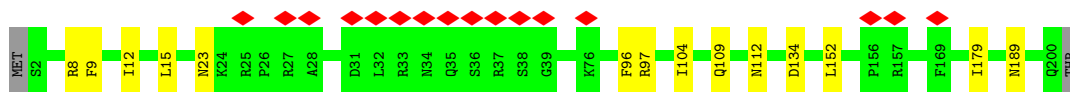
- Molecule 38: 30S ribosomal protein S2, chloroplastic



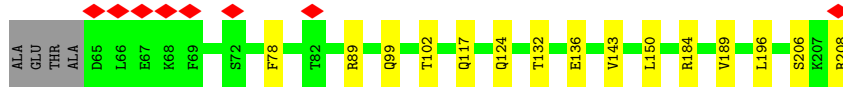
- Molecule 39: 30S ribosomal protein S3, chloroplastic



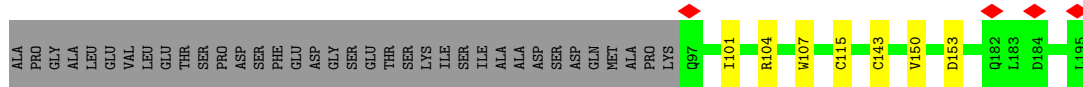
- Molecule 40: 30S ribosomal protein S4, chloroplastic



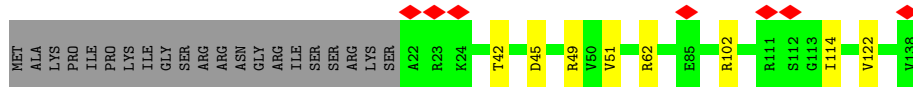
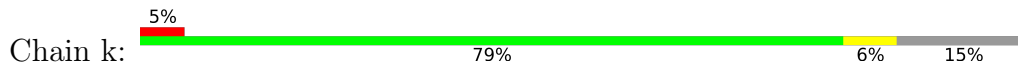
- Molecule 41: 30S ribosomal protein S5, chloroplastic



• Molecule 46: plastid ribosomal protein uS10c



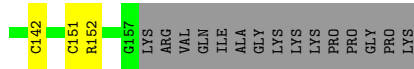
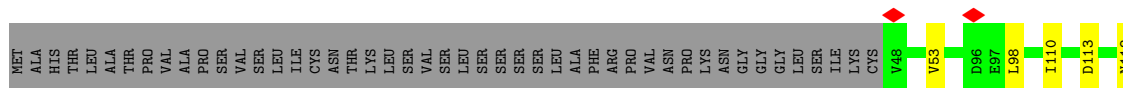
• Molecule 47: 30S ribosomal protein S11, chloroplastic



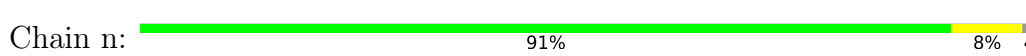
• Molecule 48: 30S ribosomal protein S12, chloroplastic



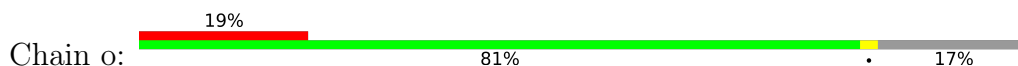
• Molecule 49: plastid ribosomal protein uS13c

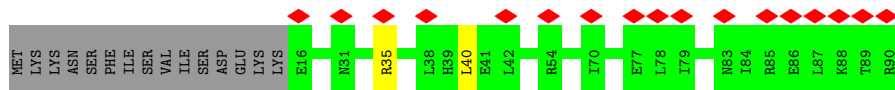


• Molecule 50: 30S ribosomal protein S14, chloroplastic

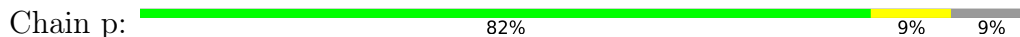


• Molecule 51: 30S ribosomal protein S15, chloroplastic

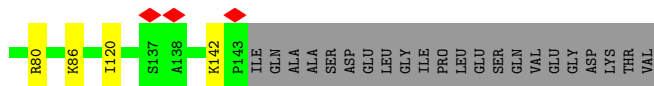
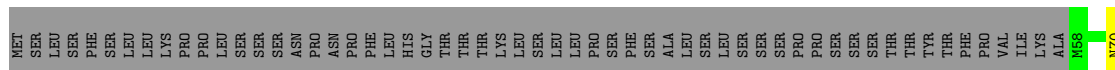




• Molecule 52: 30S ribosomal protein S16, chloroplastic



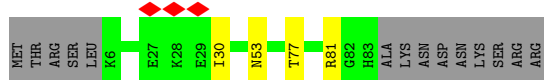
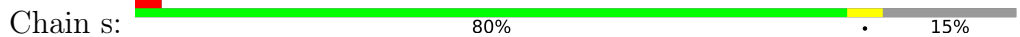
• Molecule 53: plastid ribosomal protein uS17c



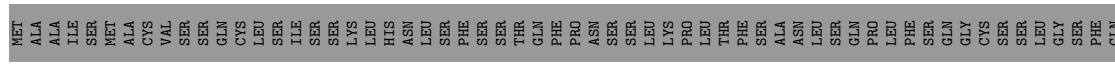
• Molecule 54: 30S ribosomal protein S18, chloroplastic



• Molecule 55: 30S ribosomal protein S19 alpha, chloroplastic



• Molecule 56: plastid ribosomal protein bS20c



• Molecule 57: plastid ribosomal protein bS21c



ASP
PRO
SER
GLN
LYS
GLU
ASP

- Molecule 61: Ribosome-binding factor PSRP1, chloroplastic



MET
ALA
THR
LEU
CYS
THR
SER
ALA
ILE
ASN
MET
ASN
PRO
ASN
LEU
THR
ASN
SER
LEU
SER
ASN
SER
ILE
ASN
LEU
SER
THR
PRO
THR
ASN
LEU
SER
PHE
THR
ASN
CYS
SER
LEU
GLY
LEU
ASN
VAL
ALA
VAL
LYS
SER
VAL
GLN
ILE
SER
ARG
ASN
LYS

PRO
ASN
VAL
VAL
CYS
MET
SER
W66
D69
G70
R82
N83
R91
R119
D122
L123
R140
R145
H181
M182
K183
GLY
PHE
ASN
ARG
SER
LYS
VAL
ARG
ASP
PRO
GLU
PRO
VAL
ARG
ILE
THR
ARG
GLU
VAL
LEU
GLU
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VAL
GLU
ASP
PRO
LYS
ASP
PHE
ILE
GLU
GLU
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VAL
ARG
THR
LYS
TYR
PHE
ASP
MET
PRO
PRO
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THR
ILE
THR
GLU
ALA
VAL
GLU
GLN
LEU
GLU
ASN
VAL
ASP
HIS
ASP
PHE
TYR
ALA
PHE
ARG
ASN
GLU
GLU
THR
GLY
ASP
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ASN
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LEU
TYR
LYS
ARG
LYS
VAL
GLY
GLY
TYR
GLY

LEU
ILE
PRO
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ASP
GLY
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THR
GLU
LYS
LEU
GLU
SER
LEU
PRO
VAL
GLN
THR
ASP
LYS
GLN
PRO
SER
PHE
ALA
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140583	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.65	0/548	0.88	1/737 (0.1%)
2	1	0.61	0/405	0.71	0/537
3	2	0.47	0/497	0.74	1/664 (0.2%)
4	3	0.55	0/470	0.71	0/619
5	4	0.57	0/594	0.67	0/784
6	5	0.38	0/307	0.54	0/403
7	6	0.46	0/425	0.77	0/551
8	7	0.43	0/382	0.57	0/520
9	A	0.82	39/67297 (0.1%)	1.21	253/104984 (0.2%)
10	B	0.49	0/2890	1.01	3/4503 (0.1%)
11	C	0.49	0/1986	0.69	2/2666 (0.1%)
12	D	0.54	0/1713	0.70	0/2291
13	E	0.54	0/1707	0.77	1/2298 (0.0%)
14	F	0.39	0/1475	0.60	1/1990 (0.1%)
15	G	0.39	0/1412	0.57	0/1898
16	H	0.41	0/386	0.59	0/514
17	I	0.54	0/1129	0.56	0/1521
18	J	0.56	0/992	0.58	0/1343
19	K	0.50	0/1688	0.63	0/2279
20	L	0.48	0/951	0.63	0/1282
21	M	0.50	0/1430	0.69	0/1896
22	N	0.45	0/1097	0.61	0/1471
23	O	0.55	0/959	0.72	0/1280
24	P	0.40	0/978	0.57	0/1311
25	Q	0.57	0/967	0.69	0/1299
26	R	0.60	0/1046	0.72	0/1395
27	S	0.48	0/1339	0.69	3/1826 (0.2%)
28	T	0.50	0/1420	0.63	0/1900
29	U	0.50	0/787	0.69	0/1056
30	V	0.42	0/1093	0.61	0/1457
31	W	0.74	0/2551	1.18	4/3977 (0.1%)
32	X	0.45	0/905	0.60	0/1204

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.46	0/644	0.62	0/856
34	Z	0.41	0/854	0.56	0/1131
35	z	1.35	7/1813 (0.4%)	1.93	81/2823 (2.9%)
37	a	0.57	0/35687	1.00	35/55680 (0.1%)
38	b	0.40	0/1878	0.55	0/2538
39	c	0.39	0/1763	0.58	0/2370
40	d	0.37	0/1661	0.57	0/2230
41	e	0.44	0/1345	0.61	0/1817
42	f	0.34	0/929	0.54	0/1255
43	g	0.37	0/1226	0.53	0/1641
44	h	0.37	0/1094	0.57	0/1467
45	i	0.37	0/1138	0.60	0/1526
46	j	0.42	0/822	0.58	0/1111
47	k	0.35	0/896	0.59	0/1206
48	l	0.45	0/975	0.60	0/1312
49	m	0.37	0/912	0.61	0/1219
50	n	0.39	0/836	0.55	0/1116
51	o	0.38	0/642	0.49	0/852
52	p	0.39	0/674	0.62	0/902
53	q	0.37	0/707	0.55	0/949
54	r	0.37	0/494	0.56	0/660
55	s	0.40	0/646	0.61	0/870
56	t	0.41	0/862	0.63	1/1151 (0.1%)
57	u	0.34	0/572	0.47	0/754
58	v	0.58	0/621	0.49	0/833
59	w	0.58	0/707	0.55	0/962
60	x	0.46	0/317	0.62	0/418
61	y	0.40	0/930	0.71	2/1243 (0.2%)
All	All	0.67	46/163471 (0.0%)	1.03	388/243348 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	E	0	1
21	M	0	1
38	b	0	1
41	e	0	1
56	t	0	2
All	All	0	6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	z	1	G	OP3-P	-10.61	1.48	1.61
9	A	1272	A	N3-C4	-8.41	1.29	1.34
9	A	1272	A	N9-C4	-7.74	1.33	1.37
9	A	727	A	N3-C4	7.72	1.39	1.34
9	A	830	A	N3-C4	-7.35	1.30	1.34
9	A	2739	A	N9-C4	-7.13	1.33	1.37
9	A	970	G	C6-N1	-7.09	1.34	1.39
9	A	1272	A	N7-C5	-6.68	1.35	1.39
9	A	772	A	N9-C4	-6.64	1.33	1.37
9	A	810	G	C6-N1	-6.25	1.35	1.39
9	A	591	C	N1-C6	-6.23	1.33	1.37
35	z	73	A	N9-C4	6.21	1.41	1.37
9	A	2044	A	N9-C4	-6.19	1.34	1.37
9	A	1399	A	N9-C4	-6.17	1.34	1.37
35	z	69	G	C6-N1	6.02	1.43	1.39
9	A	596	A	C6-N1	-5.97	1.31	1.35
9	A	727	A	N9-C4	5.91	1.41	1.37
9	A	1290	A	N3-C4	-5.90	1.31	1.34
9	A	596	A	N3-C4	-5.82	1.31	1.34
9	A	1272	A	C5-C6	-5.79	1.35	1.41
9	A	1406	A	N9-C4	-5.78	1.34	1.37
9	A	590	C	N1-C6	-5.68	1.33	1.37
9	A	180	A	N9-C4	-5.65	1.34	1.37
35	z	56	C	N1-C6	5.63	1.40	1.37
35	z	35	A	N3-C4	5.58	1.38	1.34
9	A	2051	G	C6-N1	-5.54	1.35	1.39
9	A	727	A	N1-C2	5.54	1.39	1.34
9	A	183	C	N1-C6	-5.42	1.33	1.37
9	A	805	A	N3-C4	-5.34	1.31	1.34
9	A	785	A	N3-C4	-5.34	1.31	1.34
9	A	1813	A	N9-C4	-5.33	1.34	1.37
9	A	2052	G	C5-C4	-5.30	1.34	1.38
9	A	1497	A	N9-C4	5.29	1.41	1.37
9	A	2794	A	N9-C4	-5.29	1.34	1.37
9	A	236	A	N7-C5	-5.29	1.36	1.39
9	A	469	A	N9-C4	-5.27	1.34	1.37
9	A	520	C	N1-C6	-5.23	1.34	1.37
9	A	1294	A	N9-C4	-5.22	1.34	1.37
9	A	745	A	N9-C4	-5.20	1.34	1.37
9	A	1684	C	N1-C6	-5.16	1.34	1.37
9	A	236	A	C5-C4	-5.13	1.35	1.38
35	z	69	G	N1-C2	5.11	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1374	A	N3-C4	-5.02	1.31	1.34
9	A	590	C	N3-C4	-5.01	1.30	1.33
9	A	1272	A	C6-N1	-5.01	1.32	1.35
35	z	57	G	P-OP2	-5.00	1.40	1.49

All (388) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	727	A	N1-C2-N3	-17.96	120.32	129.30
35	z	34	G	N1-C2-N2	-13.39	104.15	116.20
9	A	1272	A	C2-N3-C4	-12.32	104.44	110.60
61	y	140	ARG	NE-CZ-NH2	-11.37	114.62	120.30
9	A	727	A	C6-N1-C2	10.68	125.01	118.60
35	z	34	G	C2-N3-C4	-10.46	106.67	111.90
35	z	33	U	C5-C4-O4	-10.35	119.69	125.90
35	z	8	U	C6-N1-C2	-10.24	114.86	121.00
35	z	7	A	C8-N9-C4	9.97	109.79	105.80
9	A	1272	A	C5-N7-C8	-9.93	98.94	103.90
9	A	2122	C	C6-N1-C2	-9.77	116.39	120.30
9	A	1272	A	N1-C2-N3	9.70	134.15	129.30
35	z	34	G	N3-C2-N2	9.61	126.63	119.90
37	a	316	C	N3-C4-C5	9.47	125.69	121.90
9	A	1272	A	N7-C8-N9	9.46	118.53	113.80
37	a	1152	A	C5-C6-N1	9.30	122.35	117.70
35	z	35	A	C8-N9-C4	9.20	109.48	105.80
35	z	46	G	C8-N9-C4	-9.20	102.72	106.40
9	A	970	G	N3-C4-C5	-9.13	124.04	128.60
9	A	1272	A	C6-C5-N7	-9.12	125.92	132.30
9	A	970	G	N1-C6-O6	-8.95	114.53	119.90
37	a	316	C	C2-N3-C4	-8.94	115.43	119.90
35	z	34	G	N1-C2-N3	8.83	129.20	123.90
9	A	901	C	C2-N1-C1'	8.79	128.47	118.80
37	a	316	C	O5'-P-OP1	-8.71	97.86	105.70
37	a	1148	C	C6-N1-C2	8.62	123.75	120.30
35	z	41	C	N3-C4-C5	-8.39	118.54	121.90
9	A	1264	C	C6-N1-C2	8.36	123.64	120.30
9	A	2706	U	N3-C2-O2	-8.16	116.49	122.20
3	2	65	LYS	CD-CE-NZ	-8.14	92.98	111.70
35	z	32	U	O5'-P-OP1	-8.12	98.39	105.70
35	z	35	A	N9-C4-C5	-8.04	102.58	105.80
35	z	18	G	C8-N9-C4	8.01	109.60	106.40
35	z	42	C	N1-C2-O2	7.98	123.69	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2518	C	C6-N1-C2	-7.96	117.11	120.30
9	A	2464	G	N3-C4-N9	7.90	130.74	126.00
35	z	56	C	C6-N1-C2	-7.89	117.14	120.30
35	z	19	G	OP2-P-O3'	7.87	122.51	105.20
35	z	19	G	N7-C8-N9	-7.85	109.17	113.10
35	z	70	G	N3-C4-C5	7.83	132.51	128.60
9	A	2036	U	C5-C6-N1	-7.74	118.83	122.70
35	z	19	G	N3-C4-C5	7.73	132.47	128.60
35	z	46	G	OP2-P-O3'	7.63	121.99	105.20
37	a	1152	A	C6-N1-C2	-7.62	114.03	118.60
9	A	1184	G	C6-C5-N7	-7.61	125.83	130.40
35	z	13	C	C6-N1-C2	7.59	123.34	120.30
9	A	1000	G	N3-C4-C5	-7.51	124.85	128.60
37	a	1302	C	C6-N1-C2	-7.48	117.31	120.30
35	z	41	C	C5-C6-N1	7.45	124.72	121.00
9	A	2635	G	C8-N9-C4	7.40	109.36	106.40
9	A	2102	G	C8-N9-C4	-7.40	103.44	106.40
35	z	3	C	C6-N1-C2	-7.40	117.34	120.30
35	z	5	G	C4-C5-N7	-7.37	107.85	110.80
9	A	596	A	N1-C6-N6	-7.37	114.18	118.60
9	A	2518	C	N3-C4-C5	-7.36	118.96	121.90
9	A	802	C	N3-C4-C5	7.34	124.83	121.90
9	A	788	G	N3-C4-C5	-7.27	124.97	128.60
35	z	69	G	N3-C4-C5	7.26	132.23	128.60
37	a	316	C	C2-N1-C1'	-7.25	110.82	118.80
35	z	19	G	C8-N9-C4	7.22	109.29	106.40
9	A	901	C	C6-N1-C2	-7.20	117.42	120.30
9	A	234	C	C6-N1-C2	7.12	123.15	120.30
37	a	316	C	C5-C4-N4	-7.11	115.22	120.20
35	z	39	U	OP2-P-O3'	7.10	120.83	105.20
9	A	1650	A	C8-N9-C4	7.08	108.63	105.80
9	A	462	G	C6-C5-N7	-7.07	126.16	130.40
9	A	2294	G	C8-N9-C4	-7.07	103.57	106.40
9	A	971	U	N3-C4-C5	-7.07	110.36	114.60
35	z	7	A	N9-C4-C5	-7.07	102.97	105.80
9	A	1211	G	C8-N9-C4	7.05	109.22	106.40
35	z	70	G	N3-C4-N9	-7.02	121.79	126.00
9	A	2102	G	N7-C8-N9	7.00	116.60	113.10
9	A	2464	G	C8-N9-C1'	-6.98	117.92	127.00
9	A	901	C	N1-C2-O2	6.97	123.08	118.90
35	z	35	A	N3-C4-N9	6.96	132.97	127.40
9	A	1272	A	C8-N9-C4	-6.96	103.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	773	U	C6-N1-C2	6.95	125.17	121.00
35	z	43	C	C6-N1-C2	-6.95	117.52	120.30
9	A	1692	C	C6-N1-C2	6.94	123.08	120.30
9	A	588	A	C8-N9-C4	6.94	108.58	105.80
9	A	1334	U	N3-C2-O2	-6.93	117.35	122.20
27	S	208	ARG	NE-CZ-NH1	6.92	123.76	120.30
9	A	2063	C	C6-N1-C2	6.86	123.04	120.30
9	A	1272	A	C5-C6-N1	-6.83	114.28	117.70
35	z	45	U	C6-N1-C2	-6.83	116.90	121.00
9	A	922	U	C5-C6-N1	-6.81	119.29	122.70
35	z	18	G	N9-C4-C5	-6.78	102.69	105.40
9	A	1272	A	C4-C5-C6	6.76	120.38	117.00
9	A	773	U	C5-C6-N1	-6.73	119.33	122.70
9	A	2706	U	N1-C2-O2	6.71	127.50	122.80
35	z	65	G	N3-C2-N2	-6.71	115.20	119.90
9	A	970	G	C6-N1-C2	-6.70	121.08	125.10
35	z	44	G	C4-C5-N7	-6.70	108.12	110.80
9	A	2016	G	C8-N9-C4	-6.64	103.75	106.40
9	A	2006	G	C8-N9-C4	6.62	109.05	106.40
13	E	112	GLY	N-CA-C	-6.62	96.56	113.10
37	a	64	C	C6-N1-C2	-6.61	117.66	120.30
9	A	462	G	C4-N9-C1'	6.60	135.08	126.50
9	A	1332	G	O4'-C1'-N9	6.59	113.47	108.20
9	A	2272	G	C4-C5-N7	6.54	113.41	110.80
9	A	540	A	C4-C5-C6	-6.53	113.73	117.00
9	A	805	A	N1-C2-N3	6.52	132.56	129.30
9	A	2760	C	C6-N1-C2	6.51	122.90	120.30
37	a	316	C	C6-N1-C2	6.48	122.89	120.30
9	A	2122	C	C2-N1-C1'	6.46	125.91	118.80
9	A	1184	G	C4-C5-N7	6.45	113.38	110.80
35	z	42	C	N3-C4-C5	6.42	124.47	121.90
9	A	1684	C	C5-C6-N1	-6.40	117.80	121.00
9	A	2352	A	C8-N9-C4	-6.40	103.24	105.80
37	a	299	C	C6-N1-C2	-6.39	117.74	120.30
9	A	772	A	C2-N3-C4	-6.38	107.41	110.60
35	z	67	C	C6-N1-C2	6.38	122.85	120.30
37	a	299	C	N1-C2-O2	6.36	122.72	118.90
9	A	843	C	C6-N1-C2	-6.33	117.77	120.30
9	A	788	G	C4-N9-C1'	6.32	134.71	126.50
9	A	2533	G	N3-C4-N9	6.32	129.79	126.00
35	z	46	G	O5'-P-OP2	-6.29	100.04	105.70
9	A	2464	G	N9-C4-C5	-6.29	102.88	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	512	A	C8-N9-C4	-6.29	103.28	105.80
9	A	523	G	O4'-C1'-N9	6.27	113.22	108.20
37	a	1106	C	N3-C2-O2	-6.25	117.53	121.90
9	A	416	C	C6-N1-C2	6.21	122.78	120.30
9	A	820	G	C5-C6-N1	6.21	114.60	111.50
9	A	2073	A	O4'-C1'-N9	6.20	113.16	108.20
9	A	462	G	C8-N9-C1'	-6.19	118.95	127.00
37	a	299	C	N3-C2-O2	-6.18	117.57	121.90
9	A	2268	G	C2-N3-C4	6.18	114.99	111.90
9	A	536	C	C5-C6-N1	-6.17	117.92	121.00
9	A	514	A	N9-C4-C5	6.16	108.27	105.80
35	z	18	G	C4-C5-N7	6.15	113.26	110.80
9	A	1902	G	N3-C4-C5	-6.12	125.54	128.60
27	S	78	PRO	N-CA-CB	6.11	110.64	103.30
35	z	15	G	P-O3'-C3'	6.11	127.03	119.70
35	z	21	A	O5'-P-OP1	-6.10	100.21	105.70
14	F	57	LEU	CA-CB-CG	-6.10	101.27	115.30
9	A	2063	C	C5-C6-N1	-6.10	117.95	121.00
9	A	1290	A	N1-C2-N3	6.09	132.34	129.30
9	A	540	A	C8-N9-C4	6.07	108.23	105.80
35	z	69	G	N3-C2-N2	-6.06	115.66	119.90
9	A	788	G	N3-C4-N9	6.06	129.63	126.00
9	A	2065	U	C2-N1-C1'	-6.05	110.43	117.70
9	A	2391	C	C5-C6-N1	-6.05	117.97	121.00
35	z	8	U	C5-C6-N1	6.05	125.73	122.70
9	A	2065	U	C5-C6-N1	-6.05	119.68	122.70
35	z	69	G	C8-N9-C4	6.04	108.81	106.40
37	a	299	C	C2-N1-C1'	6.03	125.44	118.80
35	z	19	G	N3-C4-N9	-6.03	122.38	126.00
1	0	89	LEU	CA-CB-CG	6.03	129.16	115.30
9	A	2272	G	N9-C4-C5	-6.02	102.99	105.40
9	A	2349	C	C6-N1-C2	6.02	122.71	120.30
9	A	462	G	C4-C5-C6	6.01	122.41	118.80
9	A	2628	C	C6-N1-C2	-6.01	117.89	120.30
9	A	1184	G	C4-N9-C1'	6.00	134.29	126.50
9	A	1272	A	C4-C5-N7	5.99	113.70	110.70
9	A	1661	U	C5-C6-N1	-5.99	119.70	122.70
9	A	2464	G	C4-N9-C1'	5.99	134.29	126.50
35	z	34	G	OP2-P-O3'	5.99	118.39	105.20
37	a	1106	C	C2-N1-C1'	5.99	125.39	118.80
9	A	1684	C	C6-N1-C2	5.99	122.69	120.30
9	A	2437	C	C6-N1-C2	-5.99	117.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2660	G	C8-N9-C4	-5.99	104.01	106.40
35	z	67	C	N3-C4-C5	5.99	124.29	121.90
9	A	970	G	C4-N9-C1'	5.98	134.28	126.50
9	A	1184	G	C8-N9-C1'	-5.97	119.23	127.00
35	z	42	C	C6-N1-C2	5.95	122.68	120.30
9	A	525	A	C6-N1-C2	-5.95	115.03	118.60
9	A	1277	G	C4-C5-N7	5.94	113.18	110.80
9	A	2535	C	N1-C2-O2	5.94	122.47	118.90
9	A	2272	G	C5-C6-O6	-5.93	125.04	128.60
9	A	2391	C	C6-N1-C2	5.93	122.67	120.30
9	A	727	A	C2-N3-C4	5.91	113.56	110.60
9	A	901	C	C5-C6-N1	5.91	123.95	121.00
9	A	565	G	C8-N9-C1'	-5.89	119.35	127.00
35	z	70	G	N3-C2-N2	-5.88	115.78	119.90
9	A	2523	U	P-O3'-C3'	5.88	126.75	119.70
9	A	100	G	C8-N9-C4	5.87	108.75	106.40
61	y	140	ARG	NE-CZ-NH1	5.87	123.23	120.30
9	A	2505	A	C8-N9-C4	5.87	108.15	105.80
35	z	36	A	OP2-P-O3'	5.86	118.10	105.20
9	A	1264	C	C5-C6-N1	-5.86	118.07	121.00
9	A	2523	U	C5-C6-N1	5.86	125.63	122.70
35	z	19	G	C4-N9-C1'	-5.86	118.89	126.50
9	A	565	G	N9-C4-C5	-5.85	103.06	105.40
9	A	2343	C	C5-C6-N1	5.85	123.92	121.00
35	z	69	G	N1-C2-N2	5.84	121.46	116.20
37	a	316	C	N1-C2-O2	-5.84	115.39	118.90
35	z	30	G	OP2-P-O3'	5.84	118.05	105.20
9	A	588	A	N7-C8-N9	-5.83	110.88	113.80
9	A	1299	U	C5-C6-N1	-5.82	119.79	122.70
9	A	114	C	C6-N1-C2	-5.80	117.98	120.30
9	A	970	G	N3-C4-N9	5.80	129.48	126.00
9	A	1731	G	N3-C4-N9	5.78	129.47	126.00
9	A	591	C	C5-C6-N1	-5.78	118.11	121.00
10	B	29	C	C6-N1-C2	-5.78	117.99	120.30
9	A	127	C	C6-N1-C2	-5.77	117.99	120.30
9	A	919	A	N1-C6-N6	-5.76	115.14	118.60
9	A	232	G	N3-C4-N9	5.76	129.46	126.00
9	A	486	G	C8-N9-C4	5.76	108.70	106.40
9	A	802	C	C6-N1-C2	5.76	122.60	120.30
9	A	641	C	C2-N3-C4	-5.76	117.02	119.90
35	z	40	C	C6-N1-C2	5.75	122.60	120.30
9	A	1184	G	N3-C4-N9	5.74	129.44	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2610	U	C5-C6-N1	5.74	125.57	122.70
9	A	1334	U	C2-N1-C1'	5.74	124.58	117.70
35	z	42	C	C5-C4-N4	-5.73	116.19	120.20
9	A	2634	C	N3-C4-C5	-5.70	119.62	121.90
37	a	1106	C	N1-C2-O2	5.69	122.32	118.90
37	a	1106	C	C6-N1-C2	-5.69	118.02	120.30
9	A	2592	U	N1-C2-O2	5.69	126.78	122.80
37	a	29	G	C8-N9-C4	-5.68	104.13	106.40
9	A	2035	A	C8-N9-C4	5.68	108.07	105.80
37	a	166	G	N3-C4-C5	-5.68	125.76	128.60
35	z	44	G	N3-C2-N2	-5.67	115.93	119.90
9	A	1334	U	N1-C2-O2	5.67	126.77	122.80
9	A	2343	C	C4-C5-C6	-5.67	114.57	117.40
9	A	585	A	C8-N9-C4	5.66	108.06	105.80
9	A	809	A	N1-C2-N3	5.66	132.13	129.30
9	A	1977	C	C6-N1-C2	-5.65	118.04	120.30
9	A	232	G	C8-N9-C4	5.65	108.66	106.40
37	a	298	A	N9-C4-C5	5.65	108.06	105.80
9	A	565	G	N3-C4-N9	5.63	129.38	126.00
9	A	1445	G	C8-N9-C4	-5.63	104.15	106.40
9	A	1635	C	C2-N1-C1'	5.63	124.99	118.80
9	A	2159	C	C6-N1-C2	-5.62	118.05	120.30
9	A	426	C	C6-N1-C2	5.61	122.55	120.30
9	A	311	U	C5-C6-N1	-5.61	119.90	122.70
9	A	1184	G	N9-C4-C5	-5.60	103.16	105.40
37	a	687	C	C6-N1-C2	-5.60	118.06	120.30
9	A	705	U	C6-N1-C2	5.60	124.36	121.00
9	A	2507	G	N3-C4-C5	5.60	131.40	128.60
9	A	901	C	C6-N1-C1'	-5.60	114.08	120.80
35	z	27	G	O5'-P-OP2	5.60	117.42	110.70
9	A	2805	C	C6-N1-C2	-5.59	118.06	120.30
9	A	564	U	C5-C6-N1	-5.58	119.91	122.70
27	S	79	PRO	N-CA-CB	5.57	109.98	103.30
35	z	46	G	N3-C4-C5	-5.56	125.82	128.60
9	A	1160	A	C8-N9-C4	5.55	108.02	105.80
9	A	951	C	C5-C6-N1	5.55	123.78	121.00
9	A	901	C	N3-C2-O2	-5.55	118.02	121.90
11	C	231	GLY	N-CA-C	-5.54	99.25	113.10
9	A	1713	A	C5-N7-C8	-5.53	101.14	103.90
9	A	1000	G	C4-N9-C1'	5.52	133.68	126.50
9	A	2518	C	C4-C5-C6	5.52	120.16	117.40
9	A	1309	U	C5-C4-O4	5.52	129.21	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2635	G	N9-C4-C5	-5.51	103.20	105.40
35	z	70	G	P-O3'-C3'	5.49	126.29	119.70
9	A	1684	C	C2-N3-C4	-5.49	117.16	119.90
35	z	46	G	N7-C8-N9	5.48	115.84	113.10
9	A	970	G	C5-C6-N1	5.47	114.24	111.50
35	z	70	G	N1-C2-N2	5.47	121.13	116.20
9	A	591	C	C2-N3-C4	-5.47	117.16	119.90
9	A	2007	U	N3-C2-O2	-5.46	118.38	122.20
37	a	298	A	N1-C6-N6	-5.45	115.33	118.60
37	a	1043	G	O4'-C1'-N9	5.44	112.55	108.20
35	z	34	G	N9-C4-C5	-5.44	103.22	105.40
9	A	761	A	C8-N9-C4	-5.44	103.62	105.80
9	A	1400	U	N1-C2-N3	5.44	118.16	114.90
9	A	1333	U	C5-C6-N1	-5.43	119.98	122.70
9	A	1002	G	C5-C6-O6	-5.43	125.34	128.60
9	A	25	G	N1-C6-O6	-5.43	116.64	119.90
9	A	1010	C	C6-N1-C2	5.42	122.47	120.30
9	A	772	A	C5-N7-C8	-5.41	101.19	103.90
37	a	115	C	C2-N1-C1'	5.41	124.75	118.80
11	C	144	LEU	CA-CB-CG	5.40	127.71	115.30
31	W	24	C	N3-C4-C5	5.40	124.06	121.90
9	A	2077	C	C2-N1-C1'	5.39	124.73	118.80
9	A	1272	A	N1-C6-N6	5.38	121.83	118.60
35	z	70	G	OP1-P-O3'	5.38	117.03	105.20
9	A	830	A	N1-C2-N3	5.37	131.99	129.30
9	A	801	U	C5-C6-N1	-5.37	120.02	122.70
9	A	514	A	C8-N9-C4	-5.36	103.66	105.80
9	A	646	G	C5-C6-N1	5.36	114.18	111.50
9	A	970	G	N1-C2-N3	5.36	127.11	123.90
31	W	16	G	N9-C4-C5	-5.35	103.26	105.40
9	A	1497	A	C2-N3-C4	5.35	113.28	110.60
35	z	58	A	N9-C4-C5	-5.34	103.66	105.80
9	A	524	A	N1-C2-N3	5.34	131.97	129.30
9	A	2156	C	C6-N1-C2	-5.34	118.16	120.30
35	z	65	G	C4-C5-N7	-5.34	108.66	110.80
9	A	2535	C	N3-C2-O2	-5.34	118.16	121.90
9	A	1705	A	C8-N9-C4	-5.33	103.67	105.80
9	A	2520	A	C8-N9-C4	-5.33	103.67	105.80
9	A	788	G	C8-N9-C1'	-5.33	120.08	127.00
9	A	2122	C	C5-C6-N1	5.32	123.66	121.00
35	z	47	U	C6-N1-C2	5.32	124.19	121.00
37	a	1018	C	C6-N1-C2	-5.32	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2731	C	C5-C6-N1	-5.32	118.34	121.00
9	A	2075	G	C8-N9-C4	-5.31	104.28	106.40
35	z	40	C	O5'-P-OP2	-5.31	100.92	105.70
9	A	540	A	C5-C6-N1	5.30	120.35	117.70
9	A	1523	A	C8-N9-C4	-5.30	103.68	105.80
35	z	62	C	C6-N1-C2	-5.30	118.18	120.30
9	A	406	C	N3-C4-C5	5.28	124.01	121.90
9	A	745	A	C8-N9-C4	5.28	107.91	105.80
35	z	46	G	N9-C4-C5	5.28	107.51	105.40
35	z	17	C	OP2-P-O3'	5.27	116.80	105.20
9	A	1359	G	C4-N9-C1'	5.26	133.34	126.50
9	A	2065	U	N1-C2-N3	5.26	118.05	114.90
10	B	55	G	C8-N9-C4	-5.25	104.30	106.40
31	W	83	C	N3-C2-O2	-5.25	118.22	121.90
9	A	2047	A	C6-N1-C2	-5.25	115.45	118.60
9	A	2528	U	N1-C2-N3	5.25	118.05	114.90
37	a	351	G	C8-N9-C4	-5.24	104.30	106.40
9	A	1973	G	N3-C4-C5	-5.24	125.98	128.60
9	A	13	A	O4'-C1'-N9	5.24	112.39	108.20
35	z	69	G	N3-C4-N9	-5.24	122.86	126.00
37	a	166	G	C4-N9-C1'	5.24	133.31	126.50
9	A	615	G	C8-N9-C4	5.24	108.50	106.40
9	A	2294	G	N3-C4-C5	-5.24	125.98	128.60
9	A	759	G	O4'-C1'-N9	5.23	112.39	108.20
9	A	514	A	C6-N1-C2	-5.23	115.46	118.60
9	A	1635	C	C5-C6-N1	5.21	123.61	121.00
9	A	2729	A	C2-N3-C4	5.20	113.20	110.60
35	z	29	G	N3-C4-C5	5.20	131.20	128.60
37	a	1148	C	N3-C4-C5	5.20	123.98	121.90
35	z	64	A	N9-C4-C5	-5.20	103.72	105.80
35	z	5	G	C5-N7-C8	5.19	106.90	104.30
9	A	641	C	N3-C4-C5	5.19	123.98	121.90
9	A	1184	G	C5-C6-O6	-5.19	125.48	128.60
9	A	1275	A	C6-N1-C2	-5.19	115.49	118.60
9	A	2408	G	O4'-C1'-N9	5.19	112.35	108.20
35	z	40	C	N3-C4-C5	5.19	123.97	121.90
9	A	730	C	C6-N1-C2	-5.17	118.23	120.30
9	A	316	G	N3-C4-C5	-5.17	126.01	128.60
35	z	33	U	N3-C4-C5	5.17	117.70	114.60
35	z	34	G	O3'-P-O5'	-5.17	94.18	104.00
9	A	1512	U	C2-N1-C1'	5.16	123.89	117.70
9	A	462	G	N3-C4-N9	5.16	129.09	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	571	G	C8-N9-C4	5.16	108.46	106.40
9	A	2065	U	C2-N3-C4	-5.16	123.91	127.00
9	A	2229	U	C2-N1-C1'	5.15	123.88	117.70
9	A	514	A	N1-C2-N3	5.15	131.87	129.30
9	A	1206	C	C5-C6-N1	-5.14	118.43	121.00
9	A	456	C	N1-C2-N3	5.14	122.80	119.20
9	A	173	C	C6-N1-C2	-5.14	118.25	120.30
9	A	805	A	C6-N1-C2	-5.14	115.52	118.60
9	A	2036	U	C6-N1-C2	5.14	124.08	121.00
37	a	298	A	C8-N9-C4	-5.14	103.75	105.80
9	A	2739	A	C2-N3-C4	-5.13	108.03	110.60
9	A	540	A	N1-C2-N3	-5.13	126.73	129.30
9	A	112	C	C2-N1-C1'	5.12	124.43	118.80
9	A	1184	G	N1-C6-O6	5.12	122.97	119.90
35	z	43	C	N3-C4-C5	-5.12	119.85	121.90
9	A	1635	C	N1-C2-O2	5.12	121.97	118.90
9	A	2464	G	C6-C5-N7	-5.11	127.33	130.40
9	A	1988	C	C5-C6-N1	-5.11	118.44	121.00
10	B	55	G	N7-C8-N9	5.11	115.66	113.10
9	A	2272	G	N1-C6-O6	5.11	122.97	119.90
31	W	83	C	N1-C2-O2	5.11	121.97	118.90
9	A	316	G	C4-N9-C1'	5.11	133.14	126.50
9	A	1000	G	C2-N3-C4	5.10	114.45	111.90
9	A	1000	G	C5-C6-N1	5.10	114.05	111.50
9	A	28	U	C2-N3-C4	-5.10	123.94	127.00
9	A	970	G	C8-N9-C1'	-5.09	120.38	127.00
37	a	1003	C	C2-N1-C1'	5.09	124.40	118.80
9	A	58	U	N3-C2-O2	-5.09	118.64	122.20
9	A	2451	A	N1-C6-N6	5.08	121.65	118.60
9	A	2807	C	C6-N1-C2	-5.08	118.27	120.30
37	a	478	G	N3-C4-C5	-5.08	126.06	128.60
9	A	537	U	C5-C6-N1	-5.07	120.17	122.70
9	A	538	C	N1-C2-O2	5.07	121.94	118.90
9	A	592	G	C8-N9-C4	5.07	108.43	106.40
9	A	214	A	C4-C5-N7	5.06	113.23	110.70
9	A	2593	G	C4-N9-C1'	5.06	133.08	126.50
9	A	24	U	C4-C5-C6	5.06	122.73	119.70
9	A	971	U	C6-N1-C2	-5.06	117.97	121.00
56	t	172	GLY	N-CA-C	5.06	125.74	113.10
9	A	2077	C	C6-N1-C2	-5.05	118.28	120.30
35	z	9	A	OP2-P-O3'	5.05	116.31	105.20
9	A	1919	C	N1-C2-O2	5.05	121.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	z	70	G	C6-C5-N7	5.05	133.43	130.40
9	A	1055	A	C8-N9-C4	5.05	107.82	105.80
9	A	1788	U	C5-C6-N1	-5.05	120.18	122.70
9	A	830	A	C6-N1-C2	-5.04	115.57	118.60
9	A	1976	C	C5-C4-N4	-5.04	116.67	120.20
9	A	970	G	N1-C2-N2	-5.04	111.67	116.20
9	A	2034	C	C5-C6-N1	-5.03	118.48	121.00
9	A	525	A	N1-C6-N6	-5.02	115.58	118.60
9	A	2360	U	C2-N1-C1'	5.02	123.73	117.70
35	z	35	A	P-O3'-C3'	5.02	125.72	119.70
9	A	2660	G	N3-C4-C5	-5.02	126.09	128.60
9	A	2344	A	C8-N9-C4	-5.02	103.79	105.80
9	A	1000	G	N3-C4-N9	5.01	129.01	126.00
9	A	1060	A	C8-N9-C4	5.01	107.81	105.80
9	A	2069	C	O4'-C1'-N1	5.01	112.21	108.20
37	a	115	C	C6-N1-C2	-5.01	118.30	120.30
9	A	2051	G	N1-C6-O6	-5.00	116.90	119.90
9	A	457	C	N1-C2-O2	-5.00	115.90	118.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	E	134	ARG	Peptide
21	M	104	ALA	Peptide
38	b	74	VAL	Peptide
41	e	144	LYS	Peptide
56	t	173	TRP	Peptide
56	t	75	LYS	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	64/130 (49%)	56 (88%)	5 (8%)	3 (5%)	2	15
2	1	46/57 (81%)	45 (98%)	1 (2%)	0	100	100
3	2	58/66 (88%)	53 (91%)	5 (9%)	0	100	100
4	3	58/152 (38%)	54 (93%)	4 (7%)	0	100	100
5	4	70/159 (44%)	66 (94%)	4 (6%)	0	100	100
6	5	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
7	6	47/142 (33%)	46 (98%)	0	1 (2%)	7	30
8	7	44/116 (38%)	41 (93%)	3 (7%)	0	100	100
11	C	251/272 (92%)	235 (94%)	15 (6%)	1 (0%)	34	67
12	D	219/305 (72%)	206 (94%)	12 (6%)	1 (0%)	29	61
13	E	210/293 (72%)	196 (93%)	14 (7%)	0	100	100
14	F	191/258 (74%)	178 (93%)	13 (7%)	0	100	100
15	G	176/220 (80%)	165 (94%)	11 (6%)	0	100	100
16	H	46/196 (24%)	43 (94%)	3 (6%)	0	100	100
17	I	135/232 (58%)	132 (98%)	3 (2%)	0	100	100
18	J	131/224 (58%)	126 (96%)	5 (4%)	0	100	100
19	K	201/250 (80%)	193 (96%)	8 (4%)	0	100	100
20	L	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
21	M	183/271 (68%)	168 (92%)	13 (7%)	2 (1%)	14	44
22	N	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
23	O	114/126 (90%)	108 (95%)	6 (5%)	0	100	100
24	P	120/166 (72%)	113 (94%)	7 (6%)	0	100	100
25	Q	116/233 (50%)	114 (98%)	2 (2%)	0	100	100
26	R	117/128 (91%)	110 (94%)	7 (6%)	0	100	100
27	S	168/256 (66%)	158 (94%)	8 (5%)	2 (1%)	13	41
28	T	170/199 (85%)	162 (95%)	7 (4%)	1 (1%)	25	57
29	U	94/198 (48%)	89 (95%)	5 (5%)	0	100	100
30	V	132/192 (69%)	123 (93%)	9 (7%)	0	100	100
32	X	107/194 (55%)	96 (90%)	11 (10%)	0	100	100
33	Y	75/148 (51%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Z	99/168 (59%)	95 (96%)	3 (3%)	1 (1%)	15	46
38	b	231/236 (98%)	221 (96%)	10 (4%)	0	100	100
39	c	214/218 (98%)	201 (94%)	13 (6%)	0	100	100
40	d	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
41	e	185/308 (60%)	182 (98%)	3 (2%)	0	100	100
42	f	111/211 (53%)	106 (96%)	4 (4%)	1 (1%)	17	49
43	g	152/155 (98%)	146 (96%)	6 (4%)	0	100	100
44	h	131/134 (98%)	127 (97%)	2 (2%)	2 (2%)	10	36
45	i	142/208 (68%)	136 (96%)	6 (4%)	0	100	100
46	j	97/195 (50%)	93 (96%)	3 (3%)	1 (1%)	15	46
47	k	115/138 (83%)	108 (94%)	7 (6%)	0	100	100
48	l	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
49	m	108/172 (63%)	101 (94%)	6 (6%)	1 (1%)	17	49
50	n	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
51	o	73/90 (81%)	72 (99%)	1 (1%)	0	100	100
52	p	78/88 (89%)	74 (95%)	4 (5%)	0	100	100
53	q	84/165 (51%)	78 (93%)	6 (7%)	0	100	100
54	r	58/101 (57%)	55 (95%)	3 (5%)	0	100	100
55	s	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
56	t	105/183 (57%)	100 (95%)	3 (3%)	2 (2%)	8	31
57	u	63/180 (35%)	62 (98%)	1 (2%)	0	100	100
58	v	78/260 (30%)	76 (97%)	2 (3%)	0	100	100
59	w	80/179 (45%)	78 (98%)	2 (2%)	0	100	100
60	x	38/101 (38%)	37 (97%)	1 (3%)	0	100	100
61	y	114/302 (38%)	106 (93%)	8 (7%)	0	100	100
All	All	6476/9784 (66%)	6138 (95%)	319 (5%)	19 (0%)	44	72

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	92	ASP
27	S	78	PRO
49	m	53	VAL

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Mol	Chain	Res	Type
56	t	174	TYR
11	C	232	GLU
34	Z	151	SER
46	j	150	VAL
21	M	144	ARG
44	h	68	ASN
44	h	69	LYS
56	t	79	ALA
21	M	131	GLY
28	T	146	ASP
1	0	91	ALA
12	D	212	ILE
42	f	149	VAL
1	0	72	VAL
7	6	131	TRP
27	S	77	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	57/117 (49%)	54 (95%)	3 (5%)	22 52
2	1	41/50 (82%)	37 (90%)	4 (10%)	8 28
3	2	56/60 (93%)	50 (89%)	6 (11%)	6 24
4	3	50/125 (40%)	42 (84%)	8 (16%)	2 10
5	4	62/140 (44%)	52 (84%)	10 (16%)	2 10
6	5	34/34 (100%)	30 (88%)	4 (12%)	5 19
7	6	46/124 (37%)	42 (91%)	4 (9%)	10 34
8	7	40/96 (42%)	33 (82%)	7 (18%)	2 7
11	C	201/217 (93%)	185 (92%)	16 (8%)	12 38
12	D	182/259 (70%)	164 (90%)	18 (10%)	8 27
13	E	179/255 (70%)	158 (88%)	21 (12%)	5 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	F	152/214 (71%)	140 (92%)	12 (8%)	12	39
15	G	151/190 (80%)	137 (91%)	14 (9%)	9	31
16	H	42/170 (25%)	37 (88%)	5 (12%)	5	19
17	I	119/204 (58%)	109 (92%)	10 (8%)	11	36
18	J	106/189 (56%)	101 (95%)	5 (5%)	26	57
19	K	176/213 (83%)	166 (94%)	10 (6%)	20	50
20	L	101/101 (100%)	91 (90%)	10 (10%)	8	27
21	M	141/215 (66%)	123 (87%)	18 (13%)	4	16
22	N	108/108 (100%)	100 (93%)	8 (7%)	13	42
23	O	96/103 (93%)	81 (84%)	15 (16%)	2	11
24	P	100/139 (72%)	90 (90%)	10 (10%)	7	27
25	Q	104/207 (50%)	94 (90%)	10 (10%)	8	29
26	R	106/115 (92%)	93 (88%)	13 (12%)	4	17
27	S	137/223 (61%)	131 (96%)	6 (4%)	28	58
28	T	152/176 (86%)	134 (88%)	18 (12%)	5	19
29	U	85/171 (50%)	74 (87%)	11 (13%)	4	16
30	V	121/169 (72%)	111 (92%)	10 (8%)	11	36
32	X	92/163 (56%)	76 (83%)	16 (17%)	2	7
33	Y	67/130 (52%)	59 (88%)	8 (12%)	5	19
34	Z	93/153 (61%)	84 (90%)	9 (10%)	8	28
38	b	198/201 (98%)	184 (93%)	14 (7%)	14	44
39	c	186/188 (99%)	175 (94%)	11 (6%)	19	49
40	d	178/180 (99%)	164 (92%)	14 (8%)	12	39
41	e	121/255 (48%)	113 (93%)	8 (7%)	16	46
42	f	100/186 (54%)	94 (94%)	6 (6%)	19	49
43	g	125/126 (99%)	118 (94%)	7 (6%)	21	51
44	h	116/117 (99%)	108 (93%)	8 (7%)	15	45
45	i	114/169 (68%)	99 (87%)	15 (13%)	4	15
46	j	91/173 (53%)	85 (93%)	6 (7%)	16	46
47	k	91/109 (84%)	83 (91%)	8 (9%)	10	33
48	l	105/106 (99%)	98 (93%)	7 (7%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	m	99/151 (66%)	92 (93%)	7 (7%)	14	44
50	n	89/90 (99%)	81 (91%)	8 (9%)	9	32
51	o	70/85 (82%)	68 (97%)	2 (3%)	42	69
52	p	71/79 (90%)	63 (89%)	8 (11%)	6	21
53	q	77/149 (52%)	72 (94%)	5 (6%)	17	46
54	r	56/96 (58%)	51 (91%)	5 (9%)	9	33
55	s	68/81 (84%)	64 (94%)	4 (6%)	19	49
56	t	89/156 (57%)	84 (94%)	5 (6%)	21	51
57	u	59/160 (37%)	55 (93%)	4 (7%)	16	45
58	v	67/225 (30%)	67 (100%)	0	100	100
59	w	76/162 (47%)	76 (100%)	0	100	100
60	x	30/85 (35%)	30 (100%)	0	100	100
61	y	104/275 (38%)	99 (95%)	5 (5%)	25	56
All	All	5577/8434 (66%)	5101 (92%)	476 (8%)	14	35

All (476) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	51	VAL
1	0	57	LEU
1	0	59	MET
2	1	6	LYS
2	1	7	ARG
2	1	11	TYR
2	1	46	PHE
3	2	6	ASP
3	2	19	VAL
3	2	28	ARG
3	2	34	ILE
3	2	42	THR
3	2	60	ILE
4	3	97	CYS
4	3	98	LEU
4	3	115	ARG
4	3	118	MET
4	3	126	LEU
4	3	127	LEU

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Mol	Chain	Res	Type
4	3	129	ARG
4	3	142	THR
5	4	92	MET
5	4	94	THR
5	4	103	ARG
5	4	109	LYS
5	4	119	HIS
5	4	125	ASN
5	4	128	ARG
5	4	135	LEU
5	4	139	ASP
5	4	143	TYR
6	5	4	ARG
6	5	6	SER
6	5	29	ASN
6	5	36	GLN
7	6	103	LYS
7	6	118	ARG
7	6	137	LYS
7	6	138	LYS
8	7	54	LYS
8	7	62	THR
8	7	65	LYS
8	7	66	LYS
8	7	69	ARG
8	7	74	ARG
8	7	88	GLU
11	C	19	GLN
11	C	71	TYR
11	C	78	GLU
11	C	100	ILE
11	C	126	LEU
11	C	142	ILE
11	C	152	ARG
11	C	167	SER
11	C	178	ARG
11	C	188	VAL
11	C	196	VAL
11	C	203	ARG
11	C	224	VAL
11	C	228	HIS
11	C	244	THR

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Mol	Chain	Res	Type
11	C	270	ARG
12	D	109	VAL
12	D	132	ASP
12	D	137	VAL
12	D	146	ASP
12	D	174	VAL
12	D	178	ASP
12	D	193	GLU
12	D	213	LYS
12	D	221	LEU
12	D	222	MET
12	D	229	HIS
12	D	240	THR
12	D	260	LYS
12	D	262	ARG
12	D	273	LEU
12	D	288	ASN
12	D	292	LEU
12	D	298	VAL
13	E	52	LEU
13	E	61	SER
13	E	68	THR
13	E	78	GLU
13	E	97	ARG
13	E	113	ARG
13	E	120	LYS
13	E	130	ARG
13	E	147	ASP
13	E	152	MET
13	E	157	ARG
13	E	161	LEU
13	E	209	LEU
13	E	211	ASP
13	E	213	VAL
13	E	223	ILE
13	E	226	LEU
13	E	230	THR
13	E	238	ASP
13	E	245	LEU
13	E	261	VAL
14	F	56	ARG
14	F	59	THR

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Mol	Chain	Res	Type
14	F	78	ILE
14	F	88	VAL
14	F	110	LEU
14	F	119	VAL
14	F	122	LYS
14	F	127	ILE
14	F	155	ARG
14	F	164	THR
14	F	188	GLN
14	F	190	VAL
15	G	40	GLU
15	G	41	SER
15	G	50	VAL
15	G	63	LEU
15	G	94	LYS
15	G	100	ARG
15	G	102	ASN
15	G	105	HIS
15	G	109	ARG
15	G	111	LEU
15	G	127	LEU
15	G	129	LEU
15	G	169	THR
15	G	213	GLU
16	H	47	LYS
16	H	57	ILE
16	H	65	GLN
16	H	75	ARG
16	H	79	LEU
17	I	75	LEU
17	I	79	ILE
17	I	84	PHE
17	I	89	PHE
17	I	101	THR
17	I	114	VAL
17	I	119	TRP
17	I	140	ILE
17	I	147	TYR
17	I	165	CYS
18	J	90	THR
18	J	99	LEU
18	J	129	ILE

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Mol	Chain	Res	Type
18	J	152	LYS
18	J	171	ILE
19	K	48	ARG
19	K	62	ARG
19	K	64	LEU
19	K	79	LEU
19	K	82	ARG
19	K	168	ARG
19	K	169	THR
19	K	174	ARG
19	K	191	LEU
19	K	232	GLN
20	L	1	MET
20	L	2	ILE
20	L	23	ARG
20	L	25	ILE
20	L	28	SER
20	L	34	ARG
20	L	42	VAL
20	L	75	MET
20	L	102	ILE
20	L	105	GLU
21	M	83	ASP
21	M	84	ASN
21	M	106	GLN
21	M	115	ARG
21	M	120	ARG
21	M	125	ILE
21	M	127	ARG
21	M	138	ARG
21	M	150	MET
21	M	154	LEU
21	M	164	ASP
21	M	186	ILE
21	M	192	ARG
21	M	208	THR
21	M	212	ILE
21	M	215	ARG
21	M	220	SER
21	M	246	VAL
22	N	5	LYS
22	N	9	PHE

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Mol	Chain	Res	Type
22	N	28	CYS
22	N	41	TRP
22	N	44	SER
22	N	52	ARG
22	N	56	ARG
22	N	109	VAL
23	O	11	MET
23	O	19	ARG
23	O	22	ARG
23	O	27	ARG
23	O	28	ARG
23	O	36	THR
23	O	48	ARG
23	O	56	LYS
23	O	73	ARG
23	O	74	ARG
23	O	89	LEU
23	O	105	THR
23	O	111	LEU
23	O	123	ILE
23	O	126	VAL
24	P	49	ARG
24	P	52	ASP
24	P	53	ARG
24	P	59	ARG
24	P	70	ARG
24	P	87	ILE
24	P	127	ILE
24	P	143	ARG
24	P	151	ARG
24	P	161	GLU
25	Q	138	ARG
25	Q	161	ARG
25	Q	185	ARG
25	Q	198	LEU
25	Q	203	ILE
25	Q	206	ILE
25	Q	212	ARG
25	Q	215	ARG
25	Q	219	LEU
25	Q	228	ARG
26	R	6	ARG

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Mol	Chain	Res	Type
26	R	11	ARG
26	R	31	LEU
26	R	48	ARG
26	R	59	ARG
26	R	70	ARG
26	R	76	TYR
26	R	85	LEU
26	R	96	ILE
26	R	100	ILE
26	R	108	ILE
26	R	109	TYR
26	R	113	ASN
27	S	87	ASP
27	S	102	GLU
27	S	163	LEU
27	S	208	ARG
27	S	216	ILE
27	S	228	GLU
28	T	35	ARG
28	T	43	VAL
28	T	45	LYS
28	T	47	ARG
28	T	101	SER
28	T	104	GLU
28	T	110	THR
28	T	113	LYS
28	T	134	ILE
28	T	137	ARG
28	T	139	ILE
28	T	153	THR
28	T	160	LEU
28	T	163	LEU
28	T	164	MET
28	T	174	CYS
28	T	183	ILE
28	T	192	LEU
29	U	102	LEU
29	U	103	LYS
29	U	119	ILE
29	U	138	VAL
29	U	141	ARG
29	U	143	ASP

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Mol	Chain	Res	Type
29	U	154	PHE
29	U	171	THR
29	U	172	LYS
29	U	178	LEU
29	U	179	ASN
30	V	48	ARG
30	V	51	ARG
30	V	93	ILE
30	V	98	SER
30	V	130	ILE
30	V	146	SER
30	V	165	THR
30	V	171	THR
30	V	173	ASP
30	V	176	LYS
32	X	73	LYS
32	X	77	LEU
32	X	81	ILE
32	X	85	GLN
32	X	86	VAL
32	X	97	ARG
32	X	105	LYS
32	X	109	ILE
32	X	111	LYS
32	X	120	ASP
32	X	123	VAL
32	X	135	VAL
32	X	142	ILE
32	X	151	ARG
32	X	155	ARG
32	X	156	GLU
33	Y	72	ARG
33	Y	83	ASN
33	Y	87	ARG
33	Y	91	SER
33	Y	92	ASN
33	Y	98	LEU
33	Y	126	LEU
33	Y	144	ASP
34	Z	65	LEU
34	Z	74	GLU
34	Z	76	LEU

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Mol	Chain	Res	Type
34	Z	81	LEU
34	Z	87	LEU
34	Z	104	ASP
34	Z	132	LEU
34	Z	133	SER
34	Z	146	VAL
38	b	7	ASN
38	b	8	ILE
38	b	30	ARG
38	b	53	PHE
38	b	77	LYS
38	b	79	LYS
38	b	83	SER
38	b	114	ARG
38	b	119	ARG
38	b	163	ASP
38	b	175	THR
38	b	194	ASN
38	b	218	LEU
38	b	232	TYR
39	c	4	LYS
39	c	5	ILE
39	c	24	SER
39	c	42	CYS
39	c	58	GLU
39	c	78	MET
39	c	83	LEU
39	c	103	LEU
39	c	107	ASN
39	c	116	ARG
39	c	209	ILE
40	d	8	ARG
40	d	9	PHE
40	d	12	ILE
40	d	15	LEU
40	d	23	ASN
40	d	96	PHE
40	d	97	ARG
40	d	104	ILE
40	d	109	GLN
40	d	112	ASN
40	d	134	ASP

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Mol	Chain	Res	Type
40	d	152	LEU
40	d	179	ILE
40	d	189	ASN
41	e	161	ARG
41	e	187	VAL
41	e	191	VAL
41	e	210	ARG
41	e	270	LEU
41	e	272	SER
41	e	292	PHE
41	e	299	ARG
42	f	107	GLN
42	f	118	MET
42	f	119	THR
42	f	124	LEU
42	f	141	TYR
42	f	183	GLU
43	g	6	THR
43	g	10	LYS
43	g	15	ASP
43	g	25	MET
43	g	36	LYS
43	g	63	ARG
43	g	72	ASP
44	h	20	ARG
44	h	28	SER
44	h	45	ILE
44	h	46	GLU
44	h	60	VAL
44	h	76	THR
44	h	79	LEU
44	h	84	ARG
45	i	78	PHE
45	i	89	ARG
45	i	99	GLN
45	i	102	THR
45	i	117	GLN
45	i	124	GLN
45	i	132	THR
45	i	136	GLU
45	i	143	VAL
45	i	150	LEU

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Mol	Chain	Res	Type
45	i	184	ARG
45	i	189	VAL
45	i	196	LEU
45	i	206	SER
45	i	208	ARG
46	j	101	ILE
46	j	104	ARG
46	j	107	TRP
46	j	115	CYS
46	j	143	CYS
46	j	153	ASP
47	k	42	THR
47	k	45	ASP
47	k	49	ARG
47	k	51	VAL
47	k	62	ARG
47	k	102	ARG
47	k	114	ILE
47	k	122	VAL
48	l	11	THR
48	l	24	LEU
48	l	31	ARG
48	l	54	ARG
48	l	78	SER
48	l	82	VAL
48	l	101	THR
49	m	98	LEU
49	m	110	ILE
49	m	113	ASP
49	m	118	ASN
49	m	142	CYS
49	m	151	CYS
49	m	152	ARG
50	n	3	ARG
50	n	5	SER
50	n	35	THR
50	n	37	LEU
50	n	49	SER
50	n	59	LEU
50	n	68	ARG
50	n	92	LEU
51	o	35	ARG

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Mol	Chain	Res	Type
51	o	40	LEU
52	p	11	ARG
52	p	22	ILE
52	p	26	SER
52	p	28	ARG
52	p	29	GLU
52	p	33	LEU
52	p	50	VAL
52	p	66	THR
53	q	70	ASN
53	q	80	ARG
53	q	86	LYS
53	q	120	ILE
53	q	142	LYS
54	r	22	ILE
54	r	28	ILE
54	r	31	ARG
54	r	32	ASN
54	r	71	ILE
55	s	30	ILE
55	s	53	ASN
55	s	77	THR
55	s	81	ARG
56	t	99	GLU
56	t	121	SER
56	t	151	ASN
56	t	168	GLU
56	t	173	TRP
57	u	102	ARG
57	u	124	ASN
57	u	125	LYS
57	u	134	ARG
61	y	82	ARG
61	y	119	ARG
61	y	122	ASP
61	y	140	ARG
61	y	181	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	42	HIS

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Mol	Chain	Res	Type
3	2	36	GLN
4	3	143	ASN
11	C	23	ASN
11	C	149	GLN
12	D	121	ASN
12	D	215	HIS
12	D	224	HIS
12	D	288	ASN
13	E	91	HIS
13	E	118	GLN
13	E	171	ASN
14	F	60	ASN
15	G	183	GLN
16	H	42	GLN
17	I	90	GLN
17	I	130	ASN
19	K	97	ASN
20	L	92	ASN
21	M	133	GLN
23	O	18	HIS
23	O	87	HIS
24	P	81	HIS
24	P	85	GLN
24	P	93	HIS
24	P	162	HIS
26	R	37	GLN
26	R	83	HIS
26	R	99	GLN
26	R	113	ASN
27	S	108	ASN
27	S	189	GLN
28	T	97	ASN
29	U	153	ASN
30	V	180	ASN
33	Y	99	GLN
38	b	170	GLN
38	b	194	ASN
39	c	125	ASN
40	d	57	HIS
40	d	112	ASN
40	d	149	GLN
41	e	225	HIS

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Mol	Chain	Res	Type
42	f	160	ASN
43	g	20	ASN
43	g	148	ASN
44	h	19	ASN
44	h	30	ASN
45	i	81	GLN
45	i	138	ASN
46	j	117	GLN
46	j	149	HIS
46	j	151	HIS
48	l	111	GLN
49	m	52	ASN
49	m	58	ASN
49	m	66	GLN
49	m	87	ASN
49	m	145	GLN
50	n	48	GLN
50	n	53	ASN
50	n	60	HIS
50	n	81	HIS
51	o	39	HIS
51	o	43	HIS
52	p	13	GLN
53	q	98	GLN
54	r	23	GLN
54	r	79	ASN
55	s	47	HIS
55	s	69	HIS
57	u	140	ASN
58	v	258	ASN
59	w	162	GLN
59	w	168	ASN
61	y	89	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	120/121 (99%)	20 (16%)	0
31	W	105/106 (99%)	34 (32%)	1 (0%)
35	z	75/76 (98%)	22 (29%)	0
37	a	1483/1491 (99%)	349 (23%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	A	2794/2810 (99%)	658 (23%)	8 (0%)
All	All	4577/4604 (99%)	1083 (23%)	9 (0%)

All (1083) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	8	G
9	A	9	A
9	A	10	G
9	A	12	A
9	A	13	A
9	A	14	A
9	A	31	C
9	A	33	A
9	A	34	G
9	A	39	C
9	A	45	A
9	A	46	C
9	A	54	G
9	A	57	G
9	A	70	A
9	A	71	A
9	A	73	U
9	A	74	G
9	A	82	G
9	A	84	G
9	A	94	A
9	A	97	A
9	A	98	G
9	A	99	A
9	A	100	G
9	A	116	A
9	A	117	A
9	A	118	U
9	A	123	C
9	A	130	U
9	A	131	C
9	A	132	G
9	A	143	G
9	A	144	A
9	A	149	A
9	A	158	C

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Mol	Chain	Res	Type
9	A	159	A
9	A	160	A
9	A	163	G
9	A	181	A
9	A	184	A
9	A	200	G
9	A	201	A
9	A	206	A
9	A	207	A
9	A	208	A
9	A	209	G
9	A	216	C
9	A	218	A
9	A	224	G
9	A	226	A
9	A	230	G
9	A	233	G
9	A	249	C
9	A	250	A
9	A	251	G
9	A	252	C
9	A	260	G
9	A	266	A
9	A	275	U
9	A	276	G
9	A	277	G
9	A	282	G
9	A	284	A
9	A	286	U
9	A	287	A
9	A	288	C
9	A	294	U
9	A	297	U
9	A	298	G
9	A	299	C
9	A	304	A
9	A	316	G
9	A	320	U
9	A	326	A
9	A	332	G
9	A	333	A
9	A	338	G

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Mol	Chain	Res	Type
9	A	340	A
9	A	362	A
9	A	363	C
9	A	364	U
9	A	368	U
9	A	377	G
9	A	379	C
9	A	383	A
9	A	384	G
9	A	398	G
9	A	415	U
9	A	416	C
9	A	417	A
9	A	418	G
9	A	423	G
9	A	424	A
9	A	436	G
9	A	448	C
9	A	452	G
9	A	453	U
9	A	454	G
9	A	467	G
9	A	468	U
9	A	469	A
9	A	480	G
9	A	485	G
9	A	487	U
9	A	491	A
9	A	492	A
9	A	493	G
9	A	502	U
9	A	507	G
9	A	519	A
9	A	520	C
9	A	529	G
9	A	539	A
9	A	540	A
9	A	541	G
9	A	542	C
9	A	543	A
9	A	544	G
9	A	549	A

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Mol	Chain	Res	Type
9	A	554	G
9	A	557	C
9	A	558	A
9	A	559	G
9	A	560	A
9	A	561	C
9	A	565	G
9	A	573	G
9	A	582	A
9	A	583	G
9	A	585	A
9	A	593	G
9	A	597	C
9	A	609	G
9	A	610	G
9	A	612	U
9	A	613	U
9	A	614	G
9	A	623	A
9	A	630	C
9	A	632	G
9	A	633	A
9	A	635	C
9	A	639	A
9	A	643	A
9	A	645	A
9	A	646	G
9	A	649	A
9	A	657	U
9	A	658	A
9	A	664	A
9	A	665	U
9	A	667	G
9	A	675	U
9	A	680	G
9	A	681	A
9	A	688	C
9	A	696	A
9	A	697	U
9	A	701	U
9	A	713	A
9	A	722	G

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Mol	Chain	Res	Type
9	A	724	G
9	A	727	A
9	A	728	A
9	A	729	A
9	A	730	C
9	A	731	U
9	A	734	G
9	A	740	G
9	A	741	U
9	A	749	G
9	A	758	U
9	A	759	G
9	A	760	A
9	A	768	G
9	A	775	A
9	A	776	G
9	A	782	G
9	A	786	G
9	A	787	G
9	A	788	G
9	A	793	A
9	A	795	U
9	A	803	G
9	A	811	A
9	A	813	C
9	A	816	G
9	A	817	C
9	A	823	C
9	A	838	U
9	A	839	G
9	A	853	G
9	A	856	U
9	A	857	G
9	A	858	G
9	A	859	A
9	A	866	G
9	A	869	G
9	A	879	G
9	A	880	U
9	A	888	C
9	A	890	G
9	A	893	C

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Mol	Chain	Res	Type
9	A	894	G
9	A	902	G
9	A	905	A
9	A	906	C
9	A	907	C
9	A	910	A
9	A	916	G
9	A	919	A
9	A	924	U
9	A	937	U
9	A	938	G
9	A	946	A
9	A	947	A
9	A	948	U
9	A	974	G
9	A	981	G
9	A	989	G
9	A	993	C
9	A	996	C
9	A	1001	A
9	A	1002	G
9	A	1007	A
9	A	1009	A
9	A	1011	A
9	A	1017	G
9	A	1018	A
9	A	1024	A
9	A	1038	A
9	A	1039	A
9	A	1040	U
9	A	1041	G
9	A	1045	G
9	A	1050	G
9	A	1051	U
9	A	1052	G
9	A	1054	U
9	A	1055	A
9	A	1061	G
9	A	1062	G
9	A	1065	G
9	A	1070	G
9	A	1071	C

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Mol	Chain	Res	Type
9	A	1072	A
9	A	1075	G
9	A	1098	A
9	A	1099	G
9	A	1116	A
9	A	1118	U
9	A	1138	G
9	A	1140	G
9	A	1143	C
9	A	1144	U
9	A	1147	U
9	A	1155	A
9	A	1160	A
9	A	1162	C
9	A	1163	G
9	A	1166	G
9	A	1169	A
9	A	1170	A
9	A	1173	G
9	A	1190	G
9	A	1196	A
9	A	1197	A
9	A	1198	A
9	A	1199	A
9	A	1202	A
9	A	1218	G
9	A	1221	C
9	A	1226	U
9	A	1231	G
9	A	1239	C
9	A	1240	G
9	A	1241	U
9	A	1245	U
9	A	1248	G
9	A	1253	G
9	A	1254	U
9	A	1255	U
9	A	1257	G
9	A	1259	C
9	A	1261	A
9	A	1271	G
9	A	1273	G

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Mol	Chain	Res	Type
9	A	1274	A
9	A	1277	G
9	A	1289	A
9	A	1292	G
9	A	1293	C
9	A	1295	A
9	A	1296	A
9	A	1301	G
9	A	1310	C
9	A	1315	G
9	A	1321	A
9	A	1322	A
9	A	1327	U
9	A	1333	U
9	A	1334	U
9	A	1342	A
9	A	1353	A
9	A	1357	A
9	A	1359	G
9	A	1366	C
9	A	1371	C
9	A	1380	A
9	A	1381	G
9	A	1386	A
9	A	1399	A
9	A	1400	U
9	A	1402	G
9	A	1405	A
9	A	1416	A
9	A	1417	U
9	A	1423	U
9	A	1424	A
9	A	1426	U
9	A	1431	C
9	A	1432	U
9	A	1433	U
9	A	1435	U
9	A	1436	U
9	A	1437	G
9	A	1444	A
9	A	1446	G
9	A	1449	C

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Mol	Chain	Res	Type
9	A	1450	G
9	A	1456	G
9	A	1458	C
9	A	1465	A
9	A	1472	A
9	A	1476	G
9	A	1477	G
9	A	1480	A
9	A	1483	G
9	A	1484	G
9	A	1485	U
9	A	1488	A
9	A	1493	C
9	A	1494	G
9	A	1497	A
9	A	1501	G
9	A	1507	G
9	A	1513	C
9	A	1519	A
9	A	1520	A
9	A	1521	G
9	A	1523	A
9	A	1524	G
9	A	1526	G
9	A	1527	G
9	A	1528	U
9	A	1533	A
9	A	1544	A
9	A	1557	G
9	A	1558	U
9	A	1559	A
9	A	1563	G
9	A	1566	G
9	A	1568	U
9	A	1570	C
9	A	1571	G
9	A	1588	U
9	A	1594	A
9	A	1600	A
9	A	1603	A
9	A	1612	A
9	A	1620	U

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Mol	Chain	Res	Type
9	A	1621	C
9	A	1629	G
9	A	1630	G
9	A	1632	U
9	A	1633	A
9	A	1634	C
9	A	1635	C
9	A	1642	C
9	A	1643	G
9	A	1644	A
9	A	1645	A
9	A	1649	G
9	A	1666	A
9	A	1670	A
9	A	1682	C
9	A	1683	G
9	A	1684	C
9	A	1685	G
9	A	1687	G
9	A	1710	G
9	A	1711	C
9	A	1734	A
9	A	1746	C
9	A	1750	C
9	A	1760	G
9	A	1762	C
9	A	1774	G
9	A	1778	G
9	A	1783	A
9	A	1791	C
9	A	1801	A
9	A	1810	C
9	A	1812	A
9	A	1818	U
9	A	1819	A
9	A	1821	G
9	A	1826	U
9	A	1833	G
9	A	1836	C
9	A	1839	A
9	A	1849	A
9	A	1858	A

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Mol	Chain	Res	Type
9	A	1866	G
9	A	1870	U
9	A	1877	C
9	A	1882	U
9	A	1883	G
9	A	1884	A
9	A	1885	C
9	A	1900	C
9	A	1914	A
9	A	1920	G
9	A	1923	C
9	A	1926	A
9	A	1927	A
9	A	1928	C
9	A	1930	A
9	A	1931	U
9	A	1933	A
9	A	1940	U
9	A	1943	G
9	A	1944	G
9	A	1950	A
9	A	1952	A
9	A	1969	U
9	A	1974	A
9	A	1975	C
9	A	1980	A
9	A	1981	C
9	A	1984	A
9	A	1985	A
9	A	1986	G
9	A	2005	U
9	A	2006	G
9	A	2007	U
9	A	2011	G
9	A	2015	A
9	A	2017	A
9	A	2034	C
9	A	2035	A
9	A	2037	G
9	A	2044	A
9	A	2045	A
9	A	2046	G

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Mol	Chain	Res	Type
9	A	2047	A
9	A	2053	A
9	A	2057	C
9	A	2064	C
9	A	2065	U
9	A	2069	C
9	A	2073	A
9	A	2074	A
9	A	2075	G
9	A	2076	A
9	A	2077	C
9	A	2082	U
9	A	2083	G
9	A	2091	A
9	A	2102	G
9	A	2103	G
9	A	2107	G
9	A	2115	G
9	A	2116	C
9	A	2119	U
9	A	2125	C
9	A	2126	G
9	A	2127	C
9	A	2129	G
9	A	2130	C
9	A	2131	U
9	A	2132	U
9	A	2133	A
9	A	2137	G
9	A	2139	A
9	A	2140	A
9	A	2145	A
9	A	2146	A
9	A	2147	G
9	A	2148	A
9	A	2151	G
9	A	2159	C
9	A	2160	C
9	A	2161	G
9	A	2162	G
9	A	2173	G
9	A	2175	C

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Mol	Chain	Res	Type
9	A	2176	A
9	A	2177	U
9	A	2178	C
9	A	2179	A
9	A	2181	U
9	A	2182	G
9	A	2183	A
9	A	2184	G
9	A	2185	A
9	A	2186	U
9	A	2187	A
9	A	2191	C
9	A	2192	U
9	A	2193	C
9	A	2195	G
9	A	2199	G
9	A	2201	G
9	A	2202	C
9	A	2204	A
9	A	2205	G
9	A	2206	A
9	A	2209	U
9	A	2212	A
9	A	2213	A
9	A	2217	U
9	A	2219	U
9	A	2220	G
9	A	2223	A
9	A	2227	C
9	A	2229	U
9	A	2230	A
9	A	2232	G
9	A	2242	A
9	A	2243	C
9	A	2254	A
9	A	2255	G
9	A	2256	A
9	A	2260	U
9	A	2266	U
9	A	2267	G
9	A	2269	G
9	A	2296	G

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Mol	Chain	Res	Type
9	A	2297	G
9	A	2300	U
9	A	2303	A
9	A	2304	A
9	A	2305	A
9	A	2315	G
9	A	2316	G
9	A	2322	A
9	A	2323	C
9	A	2324	G
9	A	2325	G
9	A	2338	G
9	A	2339	A
9	A	2341	U
9	A	2342	G
9	A	2343	C
9	A	2344	A
9	A	2349	C
9	A	2351	G
9	A	2352	A
9	A	2364	C
9	A	2367	C
9	A	2372	C
9	A	2375	A
9	A	2378	C
9	A	2400	G
9	A	2402	C
9	A	2408	G
9	A	2419	G
9	A	2423	A
9	A	2428	A
9	A	2442	A
9	A	2444	C
9	A	2446	G
9	A	2447	A
9	A	2448	U
9	A	2452	A
9	A	2457	C
9	A	2458	U
9	A	2462	G
9	A	2464	G
9	A	2465	A

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Mol	Chain	Res	Type
9	A	2466	U
9	A	2467	A
9	A	2481	C
9	A	2487	G
9	A	2493	A
9	A	2495	A
9	A	2507	G
9	A	2508	U
9	A	2509	U
9	A	2518	C
9	A	2519	G
9	A	2520	A
9	A	2521	U
9	A	2522	G
9	A	2523	U
9	A	2524	C
9	A	2526	G
9	A	2530	U
9	A	2535	C
9	A	2542	G
9	A	2546	G
9	A	2552	U
9	A	2569	U
9	A	2571	U
9	A	2576	C
9	A	2579	U
9	A	2583	A
9	A	2584	G
9	A	2589	A
9	A	2590	C
9	A	2591	G
9	A	2593	G
9	A	2594	A
9	A	2595	G
9	A	2599	G
9	A	2601	U
9	A	2602	U
9	A	2603	C
9	A	2619	A
9	A	2625	G
9	A	2626	U
9	A	2627	C

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Mol	Chain	Res	Type
9	A	2630	U
9	A	2637	U
9	A	2640	G
9	A	2646	U
9	A	2649	A
9	A	2671	A
9	A	2672	G
9	A	2680	G
9	A	2688	A
9	A	2689	A
9	A	2696	A
9	A	2702	G
9	A	2706	U
9	A	2707	A
9	A	2708	C
9	A	2719	G
9	A	2721	C
9	A	2729	A
9	A	2740	G
9	A	2744	A
9	A	2751	A
9	A	2753	C
9	A	2762	G
9	A	2766	A
9	A	2768	A
9	A	2769	G
9	A	2770	C
9	A	2774	U
9	A	2776	A
9	A	2778	U
9	A	2783	A
9	A	2784	G
9	A	2787	C
9	A	2796	A
10	B	2	A
10	B	10	G
10	B	15	A
10	B	16	G
10	B	19	G
10	B	25	G
10	B	31	C
10	B	37	U

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Mol	Chain	Res	Type
10	B	38	C
10	B	39	C
10	B	41	U
10	B	42	C
10	B	45	G
10	B	57	U
10	B	68	G
10	B	85	G
10	B	93	C
10	B	107	G
10	B	110	C
10	B	111	G
31	W	3	A
31	W	4	G
31	W	5	A
31	W	14	G
31	W	16	G
31	W	17	A
31	W	20	C
31	W	21	G
31	W	26	G
31	W	28	U
31	W	29	U
31	W	30	A
31	W	31	U
31	W	32	C
31	W	33	A
31	W	34	U
31	W	35	U
31	W	37	C
31	W	38	G
31	W	40	U
31	W	59	C
31	W	65	U
31	W	71	C
31	W	72	A
31	W	77	A
31	W	79	G
31	W	83	C
31	W	84	C
31	W	90	G
31	W	95	A

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Mol	Chain	Res	Type
31	W	96	C
31	W	97	A
31	W	99	A
31	W	103	G
35	z	3	C
35	z	16	U
35	z	19	G
35	z	20	U
35	z	21	A
35	z	25	C
35	z	31	A
35	z	32	U
35	z	33	U
35	z	34	G
35	z	36	A
35	z	37	A
35	z	40	C
35	z	41	C
35	z	42	C
35	z	52	G
35	z	59	U
35	z	70	G
35	z	71	G
35	z	73	A
35	z	75	C
35	z	76	A
37	a	2	C
37	a	3	U
37	a	5	A
37	a	6	U
37	a	7	G
37	a	8	G
37	a	10	G
37	a	14	U
37	a	20	C
37	a	23	G
37	a	31	U
37	a	32	G
37	a	33	A
37	a	39	G
37	a	40	G
37	a	45	A

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Mol	Chain	Res	Type
37	a	48	C
37	a	49	U
37	a	50	U
37	a	52	A
37	a	53	C
37	a	55	C
37	a	60	A
37	a	70	G
37	a	72	A
37	a	73	A
37	a	74	G
37	a	76	G
37	a	77	G
37	a	78	U
37	a	82	U
37	a	83	C
37	a	85	A
37	a	88	G
37	a	90	C
37	a	103	A
37	a	104	A
37	a	105	C
37	a	106	G
37	a	113	A
37	a	114	A
37	a	115	C
37	a	127	A
37	a	130	G
37	a	135	A
37	a	142	G
37	a	147	C
37	a	152	G
37	a	166	G
37	a	167	G
37	a	174	A
37	a	179	A
37	a	180	A
37	a	183	A
37	a	188	U
37	a	191	G
37	a	196	A
37	a	211	C

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Mol	Chain	Res	Type
37	a	216	U
37	a	218	G
37	a	222	G
37	a	230	G
37	a	233	A
37	a	237	G
37	a	238	C
37	a	252	G
37	a	260	G
37	a	264	G
37	a	269	A
37	a	289	G
37	a	292	A
37	a	299	C
37	a	300	A
37	a	303	G
37	a	315	A
37	a	317	G
37	a	323	C
37	a	324	A
37	a	325	G
37	a	327	A
37	a	338	U
37	a	339	U
37	a	343	C
37	a	344	A
37	a	349	G
37	a	355	G
37	a	358	U
37	a	361	C
37	a	363	G
37	a	364	A
37	a	368	A
37	a	377	G
37	a	382	C
37	a	383	A
37	a	384	G
37	a	392	A
37	a	393	C
37	a	398	C
37	a	399	G
37	a	400	U

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Mol	Chain	Res	Type
37	a	411	U
37	a	415	G
37	a	416	G
37	a	417	A
37	a	423	A
37	a	424	G
37	a	425	C
37	a	426	A
37	a	429	G
37	a	432	G
37	a	433	G
37	a	434	U
37	a	439	G
37	a	443	A
37	a	444	A
37	a	453	G
37	a	454	G
37	a	457	A
37	a	459	C
37	a	462	U
37	a	464	U
37	a	469	G
37	a	472	G
37	a	475	G
37	a	478	G
37	a	479	U
37	a	481	A
37	a	494	A
37	a	495	A
37	a	507	A
37	a	510	G
37	a	511	A
37	a	512	U
37	a	520	A
37	a	521	A
37	a	524	C
37	a	525	G
37	a	527	C
37	a	534	U
37	a	544	A
37	a	545	G
37	a	555	A

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Mol	Chain	Res	Type
37	a	579	A
37	a	597	A
37	a	598	G
37	a	600	U
37	a	613	G
37	a	623	A
37	a	634	G
37	a	635	A
37	a	637	C
37	a	658	G
37	a	659	A
37	a	660	A
37	a	670	A
37	a	671	C
37	a	672	G
37	a	690	G
37	a	696	C
37	a	697	A
37	a	703	A
37	a	708	G
37	a	725	A
37	a	735	A
37	a	741	U
37	a	742	A
37	a	757	G
37	a	762	A
37	a	763	A
37	a	765	C
37	a	767	A
37	a	768	U
37	a	775	U
37	a	776	A
37	a	780	G
37	a	784	U
37	a	791	C
37	a	792	G
37	a	793	A
37	a	794	C
37	a	796	C
37	a	797	G
37	a	798	U
37	a	799	G

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Mol	Chain	Res	Type
37	a	821	A
37	a	844	U
37	a	863	A
37	a	875	G
37	a	876	G
37	a	883	C
37	a	891	G
37	a	909	U
37	a	915	G
37	a	918	A
37	a	920	G
37	a	921	C
37	a	924	A
37	a	925	G
37	a	926	A
37	a	941	U
37	a	942	G
37	a	943	A
37	a	944	C
37	a	945	A
37	a	948	C
37	a	953	A
37	a	958	U
37	a	961	U
37	a	963	A
37	a	966	G
37	a	969	A
37	a	972	G
37	a	973	G
37	a	974	U
37	a	975	G
37	a	976	C
37	a	978	U
37	a	979	U
37	a	980	C
37	a	981	G
37	a	982	G
37	a	985	A
37	a	986	C
37	a	992	C
37	a	1002	G
37	a	1003	C

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Mol	Chain	Res	Type
37	a	1004	A
37	a	1014	U
37	a	1019	U
37	a	1033	G
37	a	1034	U
37	a	1041	A
37	a	1043	G
37	a	1044	U
37	a	1050	A
37	a	1066	G
37	a	1073	G
37	a	1075	U
37	a	1077	C
37	a	1078	C
37	a	1079	A
37	a	1080	A
37	a	1081	C
37	a	1082	G
37	a	1084	U
37	a	1085	G
37	a	1086	A
37	a	1088	U
37	a	1089	U
37	a	1091	G
37	a	1092	G
37	a	1095	C
37	a	1099	G
37	a	1100	A
37	a	1107	U
37	a	1114	G
37	a	1115	A
37	a	1116	U
37	a	1119	G
37	a	1131	U
37	a	1132	G
37	a	1134	G
37	a	1137	U
37	a	1144	A
37	a	1145	A
37	a	1149	A
37	a	1150	U
37	a	1151	C

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Mol	Chain	Res	Type
37	a	1160	U
37	a	1161	A
37	a	1162	U
37	a	1163	G
37	a	1169	G
37	a	1174	C
37	a	1175	A
37	a	1184	A
37	a	1186	A
37	a	1187	A
37	a	1188	U
37	a	1189	G
37	a	1198	A
37	a	1204	U
37	a	1205	C
37	a	1206	G
37	a	1208	G
37	a	1217	A
37	a	1223	A
37	a	1227	A
37	a	1228	A
37	a	1229	C
37	a	1233	A
37	a	1235	A
37	a	1242	U
37	a	1244	C
37	a	1245	U
37	a	1246	C
37	a	1247	A
37	a	1248	G
37	a	1249	U
37	a	1250	U
37	a	1253	G
37	a	1265	C
37	a	1266	A
37	a	1267	A
37	a	1268	C
37	a	1270	C
37	a	1271	G
37	a	1279	G
37	a	1280	A
37	a	1301	G

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Mol	Chain	Res	Type
37	a	1311	C
37	a	1312	A
37	a	1317	G
37	a	1319	G
37	a	1322	G
37	a	1328	G
37	a	1330	U
37	a	1346	C
37	a	1347	A
37	a	1363	U
37	a	1368	G
37	a	1371	G
37	a	1378	C
37	a	1390	A
37	a	1391	C
37	a	1395	A
37	a	1400	C
37	a	1401	A
37	a	1402	A
37	a	1403	G
37	a	1404	G
37	a	1405	A
37	a	1406	G
37	a	1416	G
37	a	1417	A
37	a	1418	A
37	a	1419	G
37	a	1436	G
37	a	1440	G
37	a	1441	A
37	a	1446	G
37	a	1454	G
37	a	1455	U
37	a	1456	A
37	a	1466	G
37	a	1469	G
37	a	1478	G
37	a	1479	G
37	a	1482	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	486	G
9	A	548	G
9	A	556	C
9	A	795	U
9	A	1520	A
9	A	2035	A
9	A	2447	A
9	A	2602	U
31	W	77	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 781 ligands modelled in this entry, 781 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	8	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	1068:UNK	C	1101:UNK	N	66.30
1	8	1143:UNK	C	1201:UNK	N	11.98

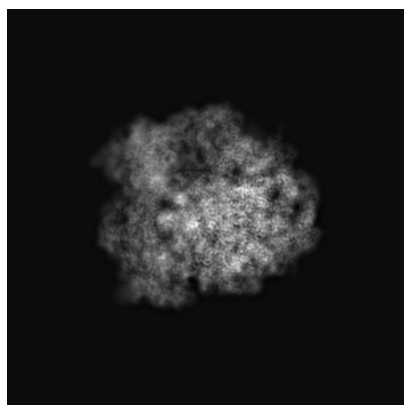
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3533. These allow visual inspection of the internal detail of the map and identification of artifacts.

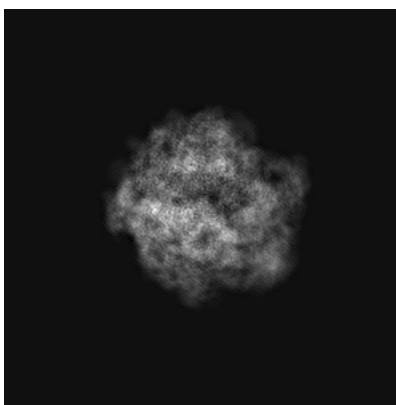
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

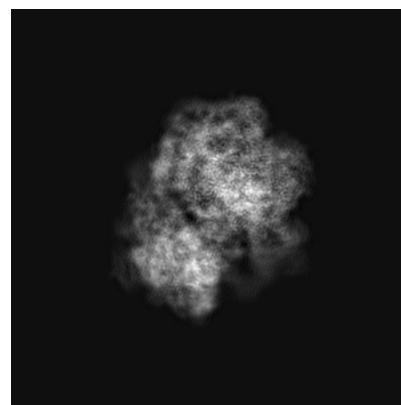
6.1.1 Primary map



X



Y

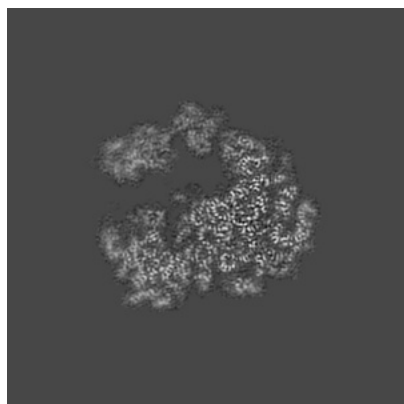


Z

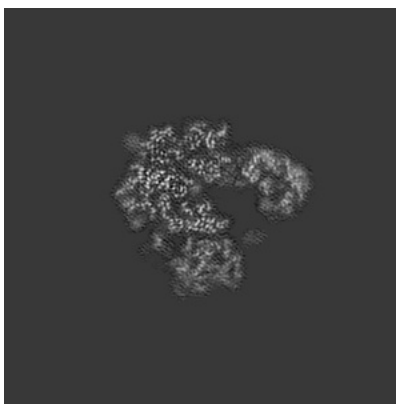
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

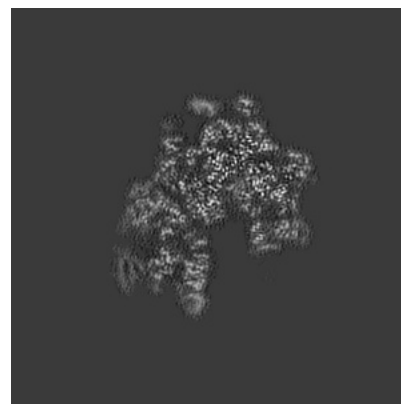
6.2.1 Primary map



X Index: 160



Y Index: 160

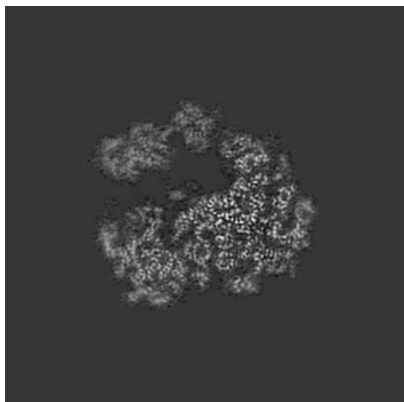


Z Index: 160

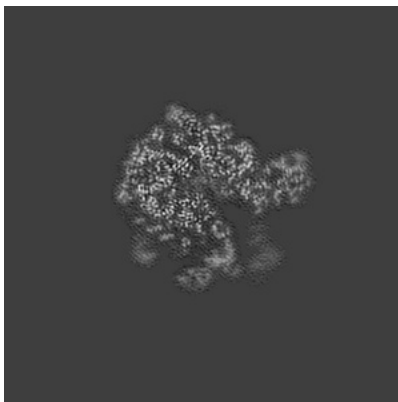
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

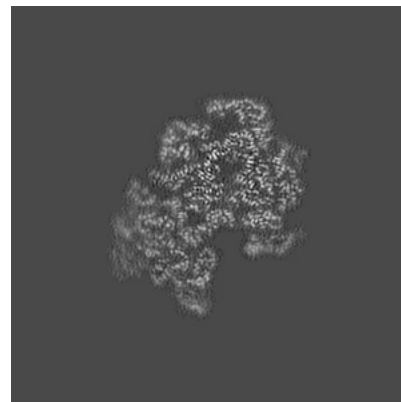
6.3.1 Primary map



X Index: 159



Y Index: 173



Z Index: 148

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

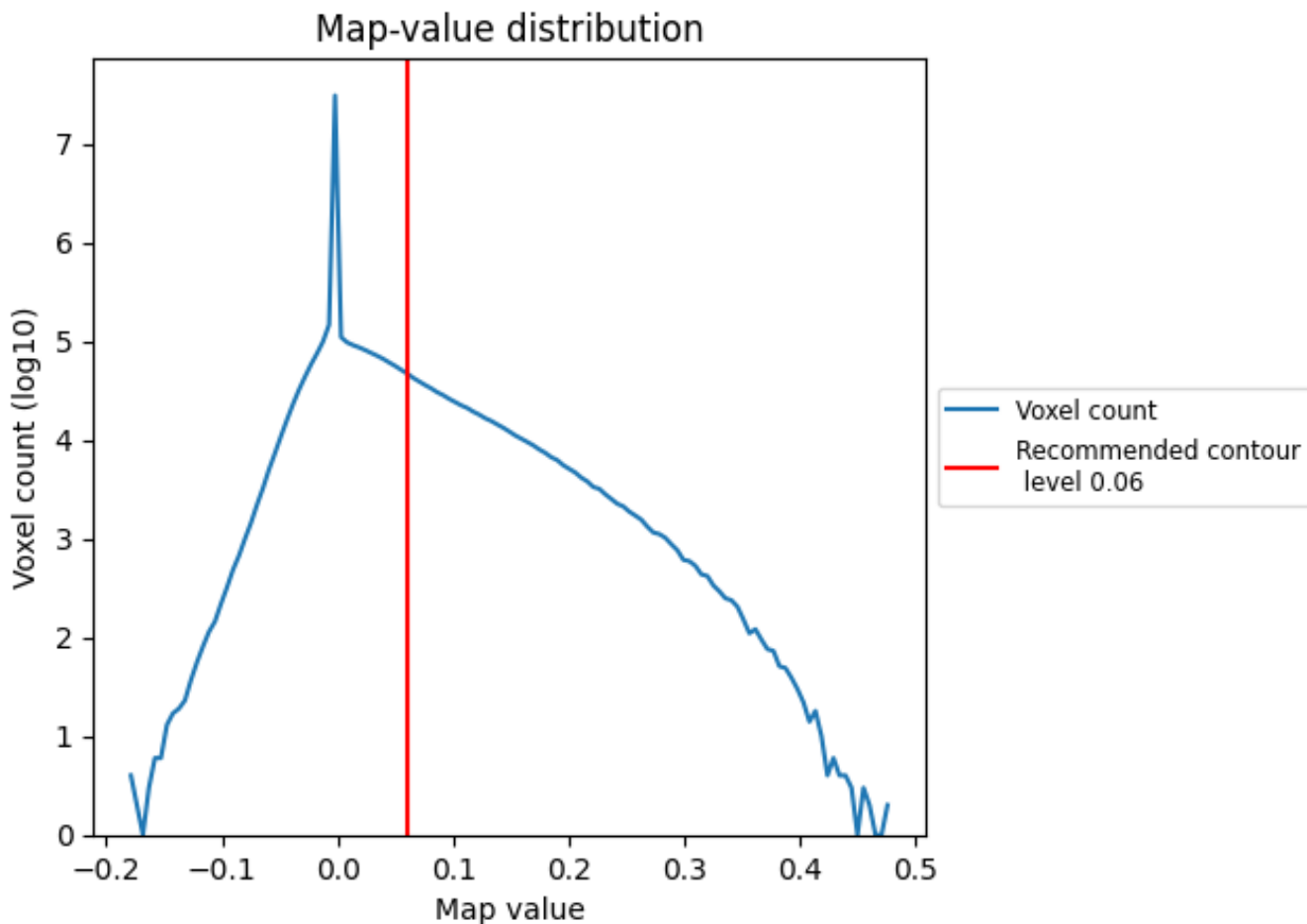
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

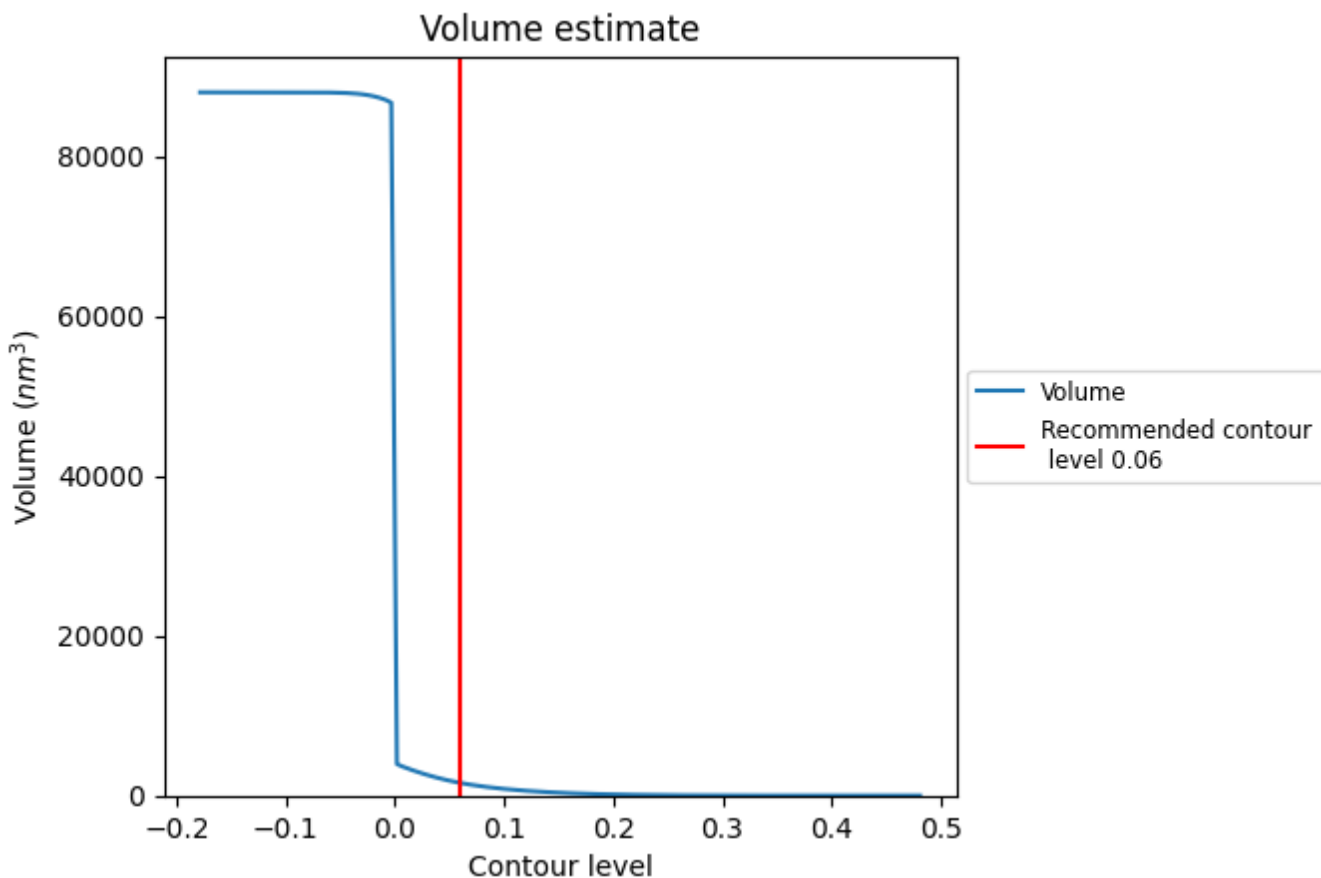
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

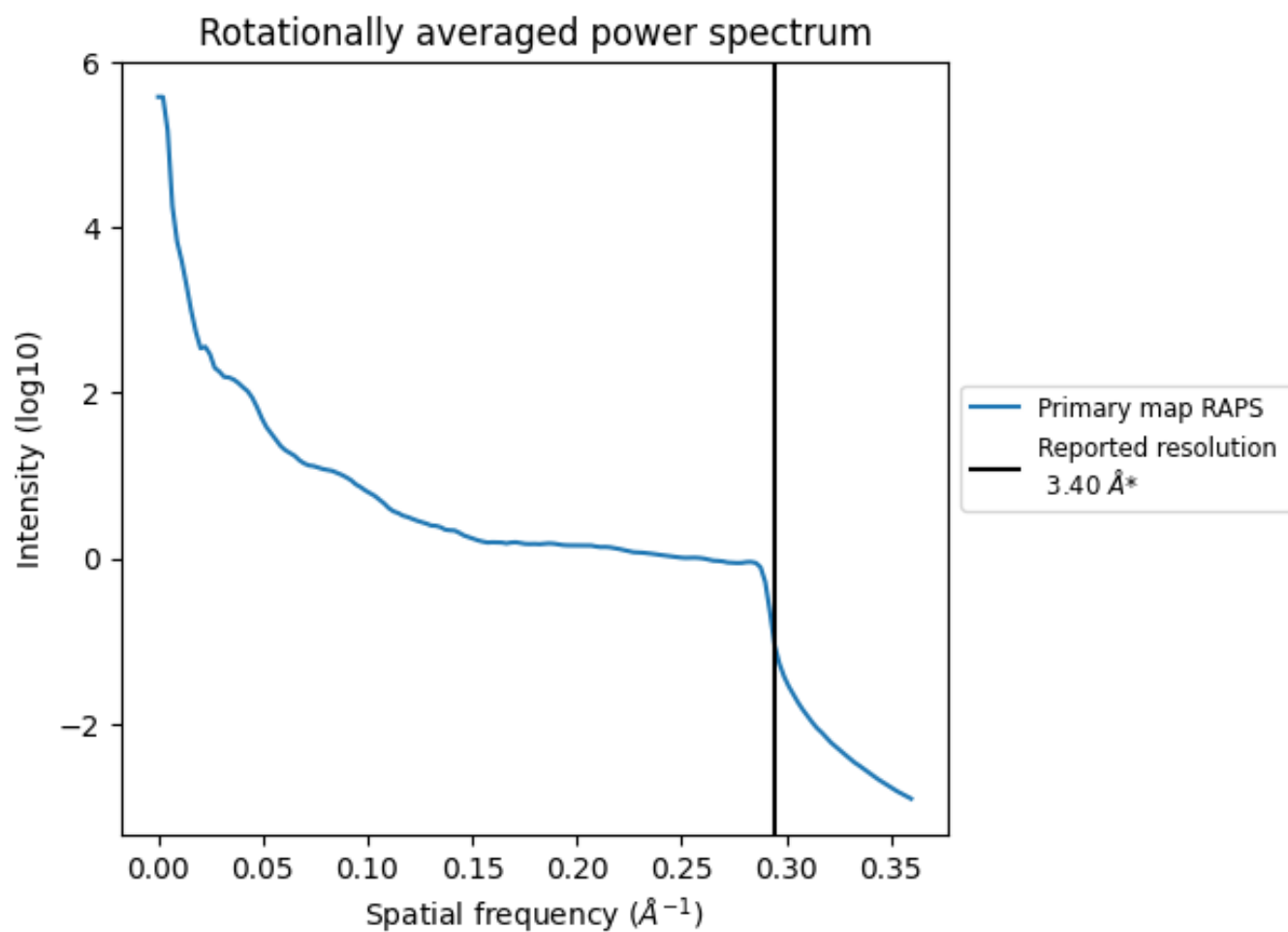
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1578 nm^3 ; this corresponds to an approximate mass of 1425 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

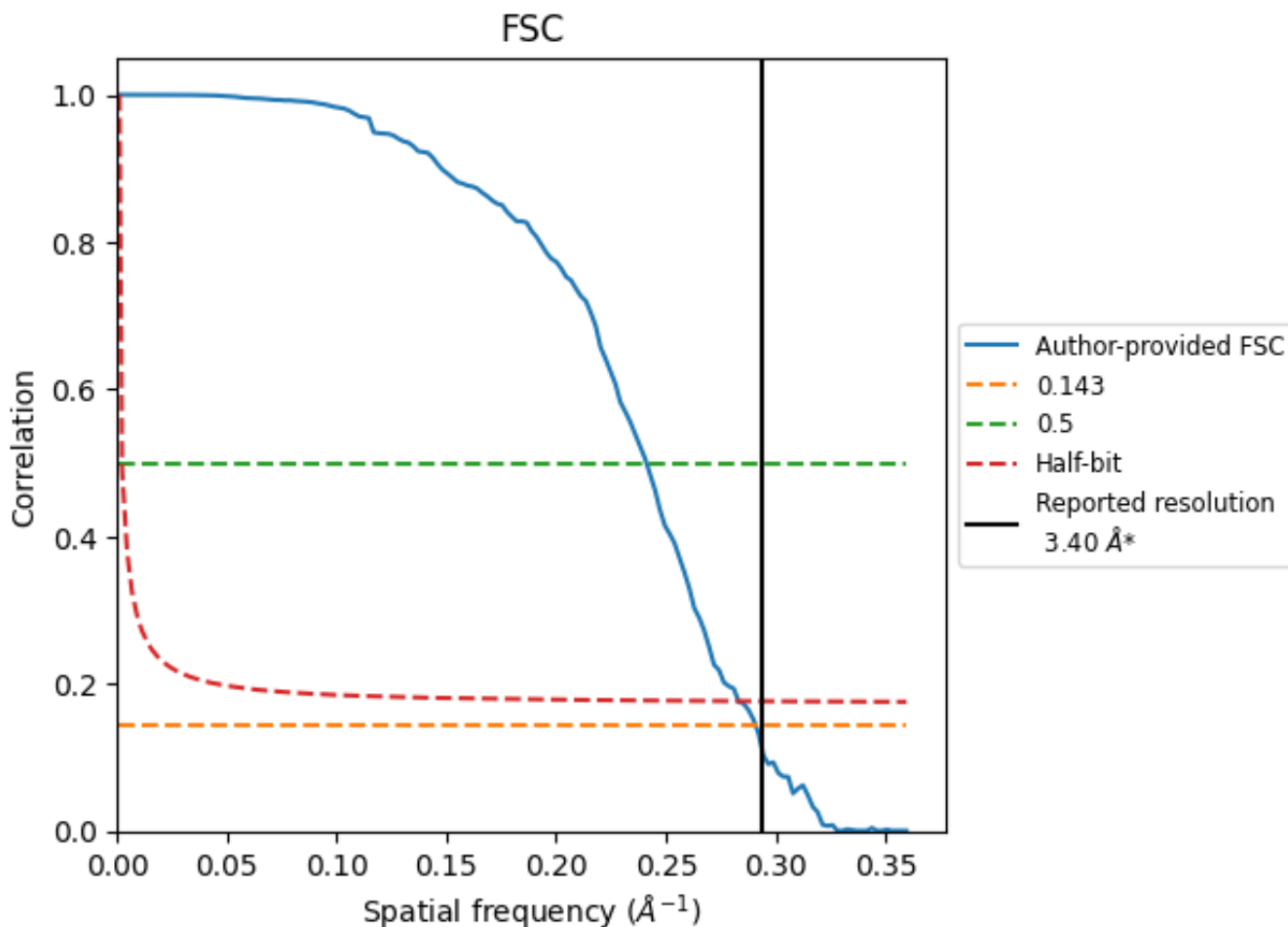


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

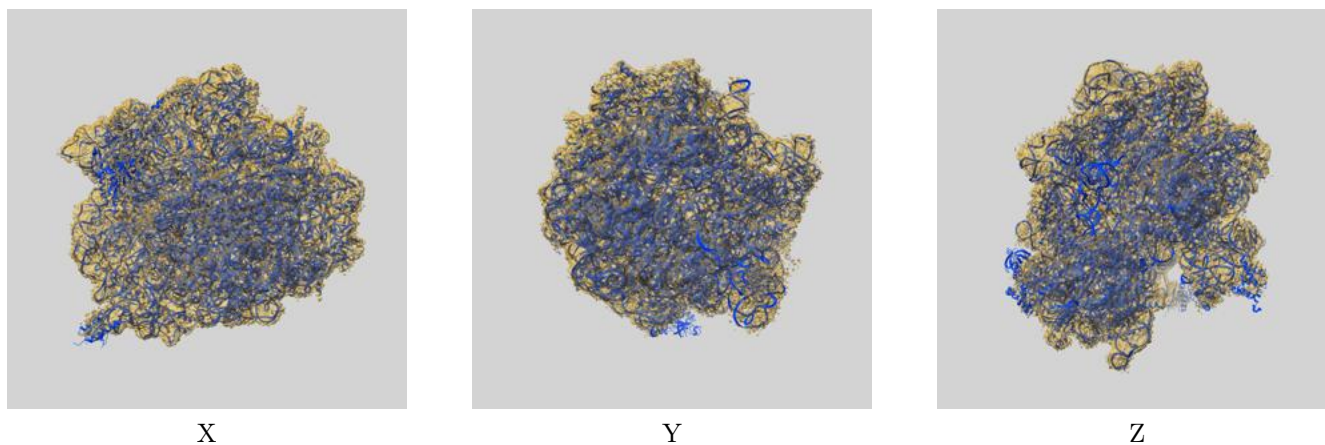
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.44	4.15	3.53
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

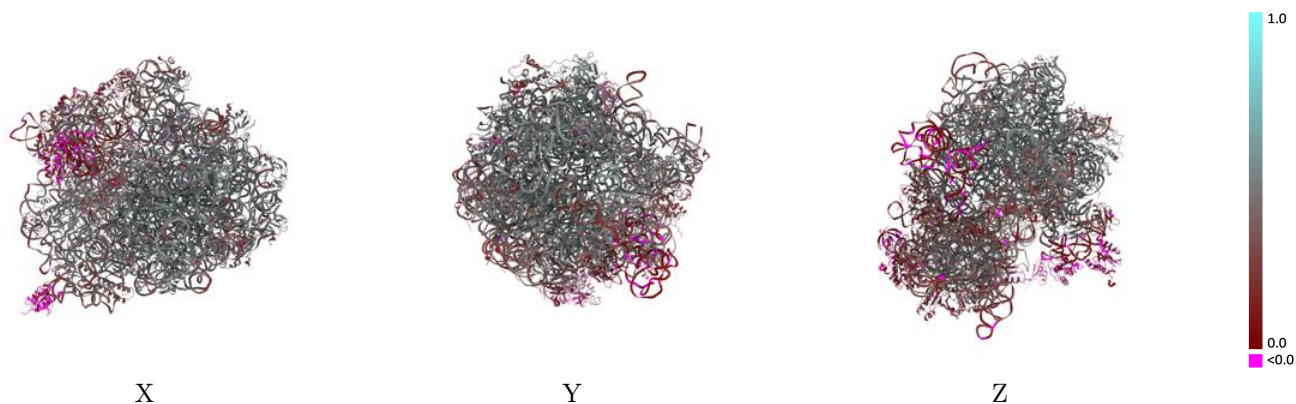
This section contains information regarding the fit between EMDB map EMD-3533 and PDB model 5MMM. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



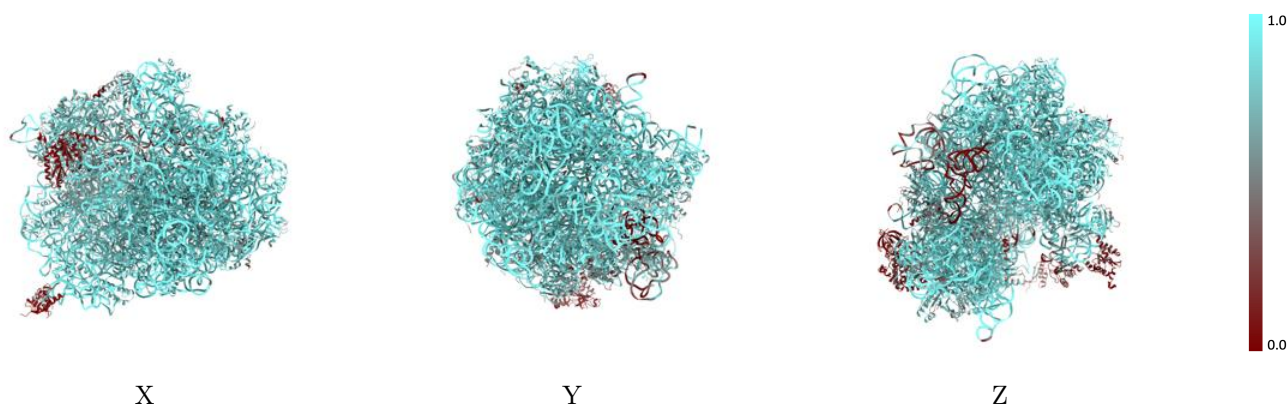
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



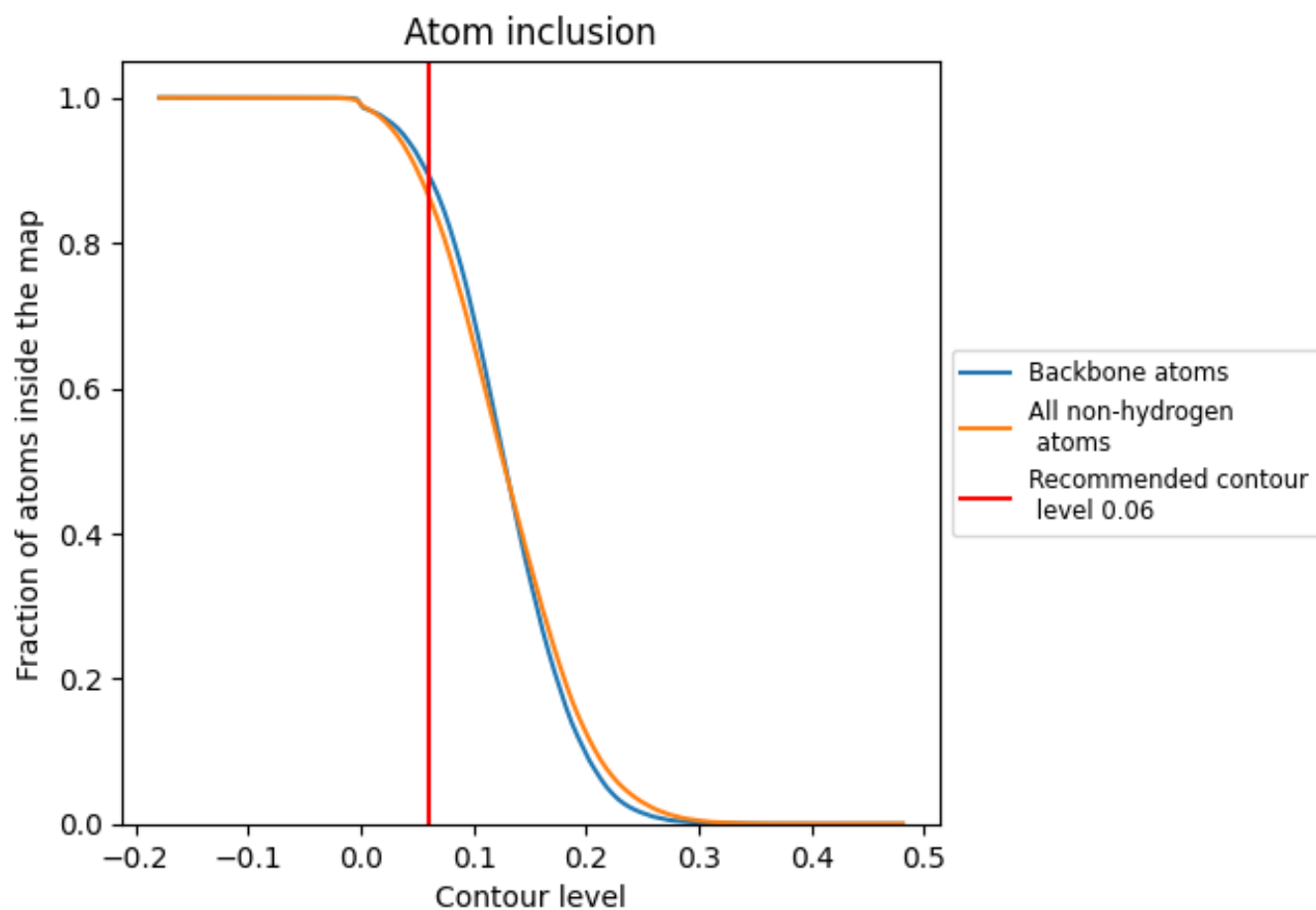
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























































The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8655	 0.4060
0	 0.5679	 0.1880
1	 0.8880	 0.4900
2	 0.8351	 0.4440
3	 0.8736	 0.5230
4	 0.8820	 0.5190
5	 0.8414	 0.4480
6	 0.7956	 0.4120
7	 0.8939	 0.4790
8	 0.0621	 0.0550
A	 0.9471	 0.4530
B	 0.9781	 0.4150
C	 0.8453	 0.4740
D	 0.8890	 0.4860
E	 0.8676	 0.4720
F	 0.7497	 0.3180
G	 0.7994	 0.3340
H	 0.5703	 0.3640
I	 0.1376	 0.0550
J	 0.2474	 0.0420
K	 0.8777	 0.4710
L	 0.8162	 0.4730
M	 0.8821	 0.4570
N	 0.6394	 0.3880
O	 0.9050	 0.4980
P	 0.8781	 0.4120
Q	 0.8477	 0.4600
R	 0.8988	 0.4970
S	 0.8359	 0.4410
T	 0.8375	 0.4460
U	 0.8200	 0.4390
V	 0.8266	 0.4310
W	 0.9747	 0.4680
X	 0.8789	 0.4610
Y	 0.8553	 0.4770



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Chain	Atom inclusion	Q-score
Z	 0.7993	 0.3890
a	 0.9670	 0.4080
b	 0.2828	 0.1970
c	 0.7353	 0.3250
d	 0.7814	 0.3520
e	 0.7446	 0.3810
f	 0.7001	 0.2920
g	 0.5709	 0.2520
h	 0.7478	 0.3400
i	 0.7888	 0.3030
j	 0.7802	 0.3140
k	 0.7793	 0.3370
l	 0.7976	 0.4510
m	 0.7592	 0.2780
n	 0.8295	 0.3360
o	 0.5635	 0.3050
p	 0.8547	 0.3850
q	 0.8027	 0.3690
r	 0.7611	 0.3150
s	 0.7528	 0.3000
t	 0.8083	 0.3470
u	 0.4496	 0.2220
v	 0.0033	 -0.0100
w	 0.1541	 0.0210
x	 0.8467	 0.3380
y	 0.6372	 0.3190
z	 0.0425	 0.0540